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THE EVALUATION OF NEUTRON NUCLEAR DATA

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REVIEW OF THE NEUTRON DATA EVALUATION ACTIVITIES, THE IMPORTANT EVALUATION NEEDS AND THE ASSESSMENT OF THESE NEEDS IN IAEA MEMBER STATES

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Abstract

On the basis of a survey performed by the IAEA the neutron data evaluation activities and needs in IAEA Member States are reviewed. The evaluation activities planned in those Member States with significant fast breeder reactor development programmes are discussed in addition to the steps being taken to facilitate the automatic conversion of data between different evaluated data libraries. The review then focusses attention on the organizational procedures which have been adopted in different States towards assessing and fulfilling their needs for evaluated data, as well as, the degree to which existing and available, evaluated data libraries satisfy the needs of users. The paper concludes by outlining the types of problems encountered in manipulating large data libraries and generating multigroup cross section sets with limited computer facilities such as exist in certain developing countries.

I. Introduction

At the outset of reviewing the neutron data evaluation activities, the important evaluation needs and the assessment of these needs in IAEA Member States it is necessary to establish an appropriate definition of what is meant by the term "neutron nuclear data evaluation". A generally accepted definition was provided by one of us [1] which states that: - Neutron data "evaluation denotes the comparison and critical assessment of the compiled experimental data and the selection by some appropriate averaging procedure

of a complete and self-consistent set of preferred values. Much more than that, the requirement of completeness, particularly for reactor physics purposes, involves the necessity of using appropriately parametrized nuclear theories and considerations of nuclear systematics to fill in gaps and to help to remove inconsistencies in the available experimental information." On the basis of this definition it is evident that the activity of neutron nuclear data evaluation forms but one element in what might be called the "neutron nuclear data cycle" which is depicted in Fig. 1. This figure reveals that the neutron nuclear data cycle may be decomposed into five basic components: - firstly, the formulation of requests for new measurements by the users of neutron data; secondly, the measurement and compilation of the experimental neutron data; thirdly, the evaluation of the compiled experimental data; fourthly, the testing of the evaluated data and the establishment and maintenance of evaluated neutron data libraries; and finally, the use of these libraries by a large user community ranging from reactor physicists and designers, shielding and safety specialists to areas such as space science and bio-medical research. In direct analogy to the situation regarding the commercial nuclear fuel cycle, it is eminently clear that only those States which are very advanced in nuclear technology can be expected to possess all of the component activities that go to make up the completely integrated neutron nuclear data cycle shown in Fig. 1. This distinction is important to bear in mind since in this paper the evaluation activities and needs of some 23 Member States, at different levels of nuclear development, are being reviewed and therefore in order to facilitate our analysis we have chosen to separately group those States with a fully integrated neutron nuclear data cycle and those without.

This review is based on the material which was supplied to the Agency in response to a Circular Letter dated 11 May 1971 (see Annex 1) which was directed to the relevant scientists in 35 Member States and replies were received from the experts in 23 States.

II. The Neutron Data Evaluation Activities in Member States with a Fully Integrated Neutron Data Cycle.

Under this item four basic questions were raised which are given in Annex II of the 11 May Circular Letter (Annex I of this review). With regard to the first enquiry concerning the neutron data evaluation activities in progress at present and those activities which will be started within the next six months, the situation is summarized in Table I in which the nuclide being evaluated, the cross section type and energy range, the Member State and

evaluator's name(s) are given. As one may expect, due to Fast Reactor Programmes a major effort is being expended in France, the Federal Republic of Germany, Italy, Japan, the U.S.A., U.K. and U.S.S.R. on the evaluation of the U-235, U-238, Pu-239, Na-23, Fe, Cr and fission product cross sections. In addition to the evaluations on Li-6, C, Cr, Mo and Pu-240 which are in progress or planned in the United Kingdom (U.K.), a considerable effort is underway there for converting a number of files for specific nuclides from the ENDF/B to the UKDNL format. A computer programme has been developed for this work and though operational it is not yet fully tested. The materials for which these conversions are being carried out are given in Table 2.1 of the paper by J.S. Story (these Proceedings).

Our second enquiry concerned the computers, the computer programmes and codes available for performing evaluations and for handling evaluated data libraries. The computers used for evaluation and handling of the evaluated data libraries are given in Table II. In particular, in the U.S.A. two computer systems have been developed for performing evaluations , namely, SCORE-II, an interactive neutron evaluation system [2] and ACSAP, an automated cross section analysis programme [3]. The evaluated neutron data libraries available in Member States are given in Table III. The principal library in use in the U.K. is the United Kingdom Nuclear Data Library (UKNDL) for which the format has been described in reference [4]. In the case of the U.S.A. the Evaluated Nuclear Data File (ENDF) was developed and is extensively used, with its format being described in the report given in reference [5]. Two different evaluated data libraries are maintained, ENDF/A and ENDF/B. The ENDF/A library contains either complete or incomplete data sets (incomplete meaning that not all major neutron cross sections for a given nuclide are contained) and it may also contain several different evaluations of the cross sections of a given nuclide. The ENDF/B library, on the other hand, contains only one evaluation of the cross sections for each material in the library, however, each material contains cross sections and related parameters for all the significant reactions. The data set which is selected for inclusion in the ENDF/B library is the set recommended by the Cross Section Evaluation Working Group (CSEWG). Another evaluated data library maintained in the U.S.A. is that of the Lawrence Livermore Laboratory (LLL). The LLL format and evaluated data file are less extensively used than the ENDF/B format and data file, however, the LLL library is up-dated semi-annually and the format is oriented to description by reaction rather than by material. While in most cases a complete evaluation is included for the isotopes or elements contained in the library, the orientation by reaction permits

inclusion of evaluations of, for example, activation reactions where the amount of material to be activated is neutronically insignificant and complete evaluations are, therefore, not required. The format of the LLL library and all relevant details are described in reference [6].

In the Federal Republic of Germany the evaluated data file KEDAK is mainly used and its format is described in reference [7]. Of these four evaluated data libraries use is made in the U.S.S.R. of the KEDAK library, whose complete contents are available to the IAEA, and certain data files of the UKNDL which are available to the Agency. Work is presently underway in the U.S.S.R. on establishing their own evaluated neutron data library on the basis of a format developed in the Soviet Union and which was described at the Soviet-Belgian-Dutch Symposium held in Melekess during February 1970, [8, 9]. With the aim of establishing this evaluated data library much effort is being spent in the U.S.S.R. on evaluating the nuclear physics characteristics for a considerable number of nuclei (given in Table I), as well as developing the necessary computer programmes for servicing, handling and using such a library.

Regarding the contents of the evaluated data libraries, ENDF/B, KEDAK, UKNDL, and the LLL these are given in Tables III. 2, III. 5, III. 1 and III. 3 respectively, of Section II.B, Annex III, of these Proceedings. The contents of the second version of the ENDF/B library as of January-February 1971 were listed in the National Neutron Cross Section Center (NNCSC) Newsletter 71-1 (1971) whilst those of KEDAK are given in reference [10]. The contents of the UKNDL library were last published in reference [11] and an indication of some of the recent additions to this library are given in Table 1.1 of the paper by J.S. Story (these Proceedings). More detailed information on the contents of these three libraries as of October 1970 is given in reference [12]. In the U.K., in addition to the extensive use of the UKNDL there is a series of programmes associated with the GENEX data library which contains tapes of resonance cross-section data in very great detail (about 120,000 energy points) over the range 0.4 eV to 25 Kev for a few fertile and fissile materials, such as, U-235, U-238; Pu-239, Pu-240 and Pu-241. These data are presented in binary format and details are given in reference [13]. The principal programmes associated with the GENEX library are RESP and GENEX. The programme RESP generates a sequence of resonance parameters by Monte Carlo selection from appropriate distributions, whilst GENEX generates Doppler broadened cross-sections for capture, fission and scattering in a standard energy mesh, using the resonance parameters supplied by RESP. As is evident from Table III, in

France, Italy and Japan, all of the three data libraries, ENDF/B, UKDNL and KEDAK are available and evaluated data produced in these countries are generated in one of these formats.

An evaluated data library requires a large number of programmes for different operations, which include, programmes for establishing, checking, editing, updating, and maintaining the library itself, processing programmes which use the data in the library (e.g. for the generation of multi-group cross-section sets) and programmes which are used to analyze and calculate cross sections during the actual process of evaluating the experimental neutron data. The computer programmes and codes which are available in Member States for the handling of evaluated data libraries are given in Table IV, whilst those for analyzing and calculating cross sections are given in Table V.

The existence of the four different evaluated neutron data libraries, ENDF/B, UKNDL, KEDAK and LLL and the present development in the U.S.S.R. towards establishing their own evaluated data library necessarily gives rise to one of the most important technical problems connected with the exchange of these libraries, namely, the conversion from one format to another. This question is dealt with in greater detail in Section II.D of these Proceedings, however, at this juncture it would be beneficial to summarize the status of the computer programmes for format conversion from one evaluated data library to another - this is done in Table VI. From this Table it is evident that considerable progress has been and is being made in overcoming the translation problem. Indeed, translation programmes now exist or are being developed for all the major libraries, except for translation from the UKNDL to KEDAK and from the U.S.S.R. format to ENDF/B, KEDAK and UKDNL. The translation programmes which have either just been completed or are nearing completion include those to translate from ENDF/B to KEDAK, from ENDF/B to UKNDL, from KEDAK to the U.S.S.R. format and from ENDF/B to the Swedish SPENG library which contains effective group and point cross sections and which is discussed below. In addition, format conversion programmes exist for translation from the UKDNL to the LLL, from LLL to UKNDL, from ENDF/B to LLL and from the LLL format to the ENDF/B format.

Our third enquiry was aimed at determining the Institutes which were involved in the evaluation effort was well as the organization and coordination of this effort between these laboratories. These Institutes are listed in Table VII and in Figs. II-V charts depicting the organization and coordination of the national evaluation effort in the U.K., France, U.S.A. and Japan are shown.

With regard to the collaboration between States in coordinating, organizing and performing evaluations, some significant progress has been made in that a partial measure of multi-national cooperation has been achieved between the E.N.E.A.* Member States through meetings of the E.A.N.D.C.** - E.A.C.R.P.***. Joint Sub-Committee on Nuclear Data Evaluation. This has so far initiated, in Europe, the series of Neutron Nuclear Data Evaluation Newsletters (NNDEN) which has been very successfully organized and edited by Dr. P. Ribon of Saclay, France. The U.K., U.S.A., Japan, Italy, Federal Republic of Germany and France all make regular contributions, on a triannual basis, to this Newsletter. In addition, this Joint Sub-Committee has been instrumental in promoting the exchange of evaluated data files between the O.E.C.D.**** Member States through the data centres at Saclay and Brookhaven. Furthermore, the Joint Sub-Committee is presently exploring whether a closer coordination of evaluation efforts can be usefully and effectively promoted, particularly in Europe, through small specialists meetings on specific topics. Added to its participation in the Joint Sub-Committee and exchanging evaluated data and test results with the E.N.E.A.* Neutron Data Compilation Centre at Saclay, the U.S.A. pointed out that the coordination of its evaluation efforts with other States is also facilitated by the bi-monthly publication of the NNCSC Newsletter.

III. The Neutron Data Evaluation Activities in Member States without a Fully Integrated Neutron Data Cycle.

For those States without a fully integrated neutron data cycle one clearly cannot expect that they will be as active in the field of evaluating neutron data as those States with a fully integrated neutron data cycle. In the cases of Argentina, Finland, Greece, Norway, South Africa, Switzerland and Turkey there are no formalized and coordinated programmes of neutron data evaluation at present or planned for the near future. Indeed, the circumstances of some of the above States were aptly summarized by Dr. G.H. Ricabarra (Argentina) when he stated that with regard to data evaluation Argentina's "position reflects more or less the situation of many developing countries, and in this sense the I.A.E.A. must be specially interested and concerned of its unique responsibility in transferring nuclear information to the developing countries, rather than being only a network center for the communication of nuclear

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* E.N.E.A. - The European Nuclear Energy Agency.
** E.A.N.D.C. - The European- American Nuclear Data Committee.
***E.A.C.R.P. - The European-American Committee for Reactor Physics.
****O.E.C.D. - The Organization for Economic Co-operation and Development.

information among the nuclearly developed countries." On the other hand, in Australia, Belgium, Bulgaria, Denmark, Hungary, India, Israel, the Netherlands, Sweden and Romania neutron data evaluations are being performed and focused on small specialized areas where it is believed that significant contributions can be made. Though work has not as yet commenced in India on the evaluation of experimental cross-section data, it is expected that a limited evaluation programme may be started in the near future. However, evaluations of "point cross sections" using the optical and statistical models have already been done at the Bhabha Atomic Research Centre for $\sigma_{n,T}$, $\sigma_{n,n}$ and $\sigma_{n,n'}$ by S.B. Garg for Cr, Fe, Ni-58, Ni-60, Mr, Cd, Pb, Th, U-235, U-238 and Pu-239 from 0.1 - 10 Mev. In the cases of Australia, Bulgaria, Hungary, Israel, the Netherlands, and Romania their present evaluation activities are summarized in Table I. In addition, evaluations on the Pu-isotopes and C may be performed in Australia in the near future but in all cases they will probably restrict themselves to 1 or 2 elements so as not to duplicate activity elsewhere. In Sweden the main effort in the area of evaluation is presently devoted to the "estimation" of the contents of the SPENG library [14] in relation to adjustments of neutron cross section data by means of least-squares fitting of the calculated quantities to the results of macroscopic experiments. This library is in free format and a description of the "element data" is given in reference [14] which describes the SPENG programme (part of the report in reference [14] is reproduced in Annex II of this Review). The library contains effective group cross sections generated by the IR approximation programme DORIX [15,16] in the 4 eV to 30 Kev region and point cross sections everywhere else between thermal energy to 15 or 18 Mev. The isotopes or elements contained in this library are given in Table 1.4 of Section II. B, Annex I, of these Proceedings.

The computer facilities available for performing evaluations and/or handling evaluated data libraries in these States are given in Table II, whilst in Table III the evaluated data libraries which are available and/or used in these States are listed. In Denmark, the Atomic Energy Commission's Research Establishment at Risø possesses a resonance parameter library - RESAB - and a 10 group fission product cross section library - FIPO. Regarding the computer programmes and codes available for evaluated data handling and the analysis and calculation of cross sections, these are summarized in Tables IV and V respectively. Although no evaluation work per se is at present in progress in Belgium, they have concentrated their efforts on translating

existing data libraries from one format to another and have just completed a converion programme to translate from the ENDF/B to the KEDAK library. Similarly in Sweden a conversion programme, ETOS, has just been completed to translate from the ENDF/B to the SPENG library. The Institutes in those states without a fully integrated neutron data cycle are given along with those in states with a fully integrated neutron data cycle in Table VII, and in Figs. VI and VII the charts showing the organization of evaluation activities in Australia and Sweden respectively are shown.

Concerning the bilateral or multilateral collaboration between these states in coordinating and performing evaluations, Australia indicated that though evaluated data have been obtained and exchanged on bilateral basis as part of general bilateral agreements, it has no formalized collaboration agreements concerning data evaluations. Australian staff have, however, contributed to evaluations done in other states during an attachment to some group in those countries. The Soreq Nuclear Research Centre (Israel) has an active collaboration with the Kernforschungszentrum Karlsruhe through a research contract which includes the complete evaluation of Pu-240, Pu-241 and Pu-242 cross sections for the KEDAK library. In the case of Sweden, it participates in the E.A.N.D.C. - E.A.C.R.P. Joint Sub-Committee of Neutron Data Evaluation and contributes to the NNDEN Newsletter. Furthermore, Sweden indicated that though their evaluations are often documented as internal reports, these as well as copies of files of the SPENG library would be made available on request. The other Scandinavian countries, Norway, Denmark and Finland participate in the annual meetings of the Scandinavian Data Committee thereby exchanging information in the field of nuclear data. On the other hand, Bulgaria participates with other States through the Joint Institute of Nuclear Research (JINR) at Dubna and the Council for Economic Aid for East-European Countries, whilst the Reactor Centrum Nederland has informal contacts with the Centro di Calcolo at Bologna, Italy. However, for the other States, Belgium, India, Turkey, Greece and South Africa there is no bilateral or multilateral collaboration in coordinating and performing evaluations due, in large part, to the fact that no evaluations per se are presently being performed in these States.

IV. The Important Neutron Data Evaluation Needs and the Assessment of these Needs in Member States.

The needs for evaluated neutron data and the necessity to perform evaluations clearly depend on a nation's programme as well as on the adequacy of the available and existing evaluated neutron data. It is furthermore evident that central to the question of assessing both the needs for performing evaluations and for evaluated data is that of, who are the users of evaluated neutron data. These users cover a broad spectrum of disciplines, however, the replies from virtually all States indicated beyond doubt that the most important group of users were the thermal and fast reactor physicists and engineers, as well as reactor design personnel. Added to this body of users were those physicists engaged in shielding, dosimetry and radiation damage calculations, the health and safety specialists and scientists involved in fuel-element fabrication and testing. Nuclear physicists involved in both experimental and theoretical work formed yet another large group of users, as did space scientists, bio-medical researchers and those engaged in developing techniques and instruments for nuclear safeguards. In addition to these user groups the U.K. pointed out that recently fusion reactor physicists have begun to use the UKNDL and also to make contriubtions to it.

Regarding the assessment of the neutron data evaluation requirements within states, for Japan the proolems associated with evaluation activities are assessed at meetings of the Japanese Nuclear Data Committee (JNDC) which acts as a Steering Committee so that the requirements for evaluation are discussed, assessed and identified by the Evaluation Working Group of the JNDC.

In contrast, in the Federal Republic of Germany requests for evaluations are usually given directly to the evaluation group at Karlsruhe. The existing evaluated data libraries and available evaluations are then checked as to whether or not they fulfil the requirements specified by the requestors. The remaining requests are then reviewed and assigned priorities, this being done in close collaboration with the main users of evaluated data in Germany. In assigning priorities to requests for evaluations account is taken not only of the importance, urgency and amount of evaluation work which may be involved, but also of the evaluations planned or in progress at other Institutes and, in this context, the Newsletters NNDEN and that of the NNCSC are felt to be of special usefulness.

In the U.S.S.R. the requirements and needs for the evaluation of neutron data are determined by the Nuclear Data Centre (Centr po Jadernym Dannym) at

Obninsk in collaboration with the laboratories responsible for reactor and shielding calculations. The requests which are submitted to the Nuclear Data Centre are then considered and approved by the USSR Central Nuclear Data Commission and its Sub-Group on Data Requirements. Methods are presently being devised for determining the data needs and two papers [17,18] have recently been published in this connection. Furthermore, the Nuclear Data Commission and the Nuclear Data Centre bear the main responsibility for organizing and coordinating the evaluation work between the various U.S.S.R. Institutes. In France, requests for evaluations are first compiled by the group in charge of evaluation and then examined, on a national basis, by the Committee on Nuclear Data, and are subsequently compiled for all Euratom States and re-examined within the Joint EURATOM Nuclear Data and Reactor Physics Committee (JENDRPC). For the U.S.A. data requirements are not always neatly separated into evaluations and measurements. The measurement requests are sent to the A.E.C.'s Neutron Cross Section Advisory Committee (NCSAC) and are reviewed for possible inclusion in the international request list, RENDA. However, evaluation requests are sent to the Chairman of the Cross-Section Evaluation Working Group (CSEWG) and are subsequently reviewed for possible inclusion in the CSEWG evaluation programme. In addition, some evaluations are requested and performed in channels other than CSEWG and, in particular, most requests for evaluations and evaluations performed at LLL originate in other than CSEWG channels.

In the case of the U.K. there are at present three bodies concerned with differential nuclear data. The Nuclear Data Working Party (NDWP) which meets on an ad hoc basis to collate and screen the U.K. nuclear data Request List so as to keep it up-to-date and make recommendations on the priorities of new differential measurements. This body acts in an advisory capacity to the Physics of Reactors Research Committee which is responsible for the formal approval of the Request List and for the evaluation/measurement programme. The Nuclear Data Files Working Party (NDFWP) on the other hand, has the main task of coordinating the U.K. evaluation work, particularly as it applies to the generation of computer files of nuclear data. The third body is the U.K. Nuclear Data Committee (UKNDC) whose main task is the coordination of the differential data measurement programme. This Committee also organizes an annual Nuclear Data Forum, a one day symposium, which convenes at each of the centres of measurement or user activity. As a result of the increased use of and the development of the UKNDL, users' requirements for new neutron data are

most frequently requirements for new or revised evaluations in the standard UKNDL format. New experimental data may also be needed but provision of these goes only part of the way towards meeting the users' requirements. This has therefore resulted in a shift of emphasis towards new evaluation work even at the expense of new measurements. Simultaneously, their Request List has now been split into two parts relating to new measurements on the one hand, and new evaluation requirements on the other. The methods whereby the accuracy requirements for cross-section data for thermal and fast reactors were determined were given in the papers in references [19,20]. However, since some of the most important cross sections cannot yet be measured to sufficient accuracy by differential methods, it has been felt necessary to institute a programme for data adjustment which takes account of both differential and integral data and their uncertainties to improve the accuracy of fast reactor performance predictions. This development has alleviated the demands for differential cross-section data of very high precision and is described in the paper by Campbell and Rowlands given in reference [21].

Most of the other States which need evaluated data essentially go about identifying their neutron data evaluation requirements in the manner outlined above for France, the Federal Republic of Germany, Japan, U.K., U.S.A. and U.S.S.R., though the procedures and channels employed for this purpose are primarily ad hoc and not on a formalized basis. In the case of Sweden their evaluation requirements mainly arise from AB Atomenergi (A.E.) and the Research Institute of the Swedish National Defense (F.O.A.). Within AB Atomenergi these requirements are forwarded to the Cross Section Data Committee where they are discussed and eventually the need for a new evaluation is assessed, however, the F.O.A. usually satisfies its own requests for evaluations. An A.E. - F.O.A. Contact Group on cross sections and basic nuclear data has recently been established and the data evaluation needs will be discussed within that Group. Other organizations in Sweden which use evaluated data are Vattenfall, Oskars-Lamns Kraftgrupp AB and Asea-Atom, though they mainly require data in group structures and these are generally furnished to them by AB Atomenergi.

Our final question was aimed at determining the degree to which the existing evaluated data libraries satisfied the needs of the users in each State, as well as the needs for evaluated data in those States that

do not possess a neutron data evaluation programme. In this context, the U.S.S.R. pointed out that since the existing evaluated libraries are accessible to U.S.S.R. scientists only partially and not in up-dated form, it was very difficult to judge to what extent these libraries satisfied the needs of those in the U.S.S.R. requiring evaluated data in their work; however, it could be stated that probably their current needs were only satisfied to a very limited extent and therefore, the U.S.S.R. was establishing its own evaluated data library. In the case of Italy, it was felt that for thermal reactors the completeness of the existing libraries was good and regarding the accuracy of the data, this was satisfactory. However, for fast reactors the completeness was fairly good but the accuracy was unsatisfactory, particularly in the few Kev and few Mev energy regions for almost all nuclei of interest. The reply from the U.S.A. indicated that a definite and objective answer to the question of the degree to which the existing libraries met the users' needs was probably not possible. This was especially due to the fact that an analysis of this question is complicated by the fact that the needs of users and the data files available are continually changing with time. However, the rate at which the data needs were defined appeared to be reasonably well matched by the rate at which new evaluations were undertaken. In the case of the Federal Republic of Germany, the existing data libraries meet the needs of their users as far as quantity is concerned, with the exception of requests for nuclear data of a number of actinides and some fission products which are fulfilled neither by the existing libraries nor by existing evaluations. Since the majority of German users of evaluated data depend on the processing programmes, such as for the generation of group constants, they are restricted to the contents of the KEDAK library. This therefore means that requests for evaluations arise both from the limited number of materials available in the KEDAK library and also from the inadequate quality of some of the data contained in the library. The first problem can be overcome by incorporating into the KEDAK library some of the evaluated data sets originating from other libraries and this therefore will necessitate a close collaboration between the evaluators. However, regarding the second problem, the inadequate quality of the evaluated data stored in the KEDAK library, this must be attributed to the lack of sufficient manpower to regularly update the contents of the library. In his reply, Dr. P. Ribon (France) noted that the existing evaluated libraries meet the needs of

French reactor physicists up to a certain point, but they still wished to have much better accuracy for these data. However, the needs of those involved in shielding studies were often very badly satisfied by the existing libraries, since when an evaluation is being performed to satisfy reactor needs one aims at establishing a good value of $\langle \sigma \rangle$, whereas, for shielding, one needs a good value for $\langle 1/\sigma \rangle$. Furthermore, because of the very varied nature of requests for evaluated data originating from those involved in the field of dosimetry, their needs were inadequately satisfied.

For the U.K., Mr. J.S. Story indicated that data files are available in the UKNDL for almost all materials of current interest for the U.K. reactor programme. Considering the most important materials, the evaluations are up-to-date to within about 1 year and the accuracy of this group of data files is essentially limited by the uncertainties in the basic experimental data, at least for the principal reactions. However, multi-group cross-section sets in up to 2000 groups have been and are being produced from these files and are usually adjusted to give improved agreement with integral experiments. In Table 1.1 of the paper by J.S. Story (these Proceedings) a rather detailed review of the degree to which the UKNDL meets the current needs of U.K. users is given. The data files for some structural materials still are in need of improvement, for example, for Cr and Mo. In addition, many files of fission-product capture cross-sections are available, but have not yet been extensively tested; many of these files require improvement and there is a need for average data on other reactions in bulk fission products, elastic and inelastic scattering for example, and perhaps also for the (n,p) and (n, α) reactions.

In the case of Japan it is considered that the existing evaluated data files are satisfactory for reactor design up to about 75%, however, neutron data for nuclides such as Ar-40, Co-59, Np-239 and the fission product nuclides are either not found or are unsatisfactory in the existing evaluated data libraries. In addition, not only is the accuracy of the existing evaluated data for the heavy nuclides not sufficient to meet the needs of the users, but there is no existing evaluted neutron data file including such data as γ-ray spectra from (n, γ) and (n, n'γ) reactions which are required for shielding calculations.

The degree to which the needs for evaluated data are met by the existing data libraries was one of the questions presently under discussion in Sweden in the Joint AB Atomenergi - F.O.A. Contact Group. Generally, the updating of existing evaluated cross sections is undertaken at AB Atomenergi in connection with adjustments resulting from macroscopic experimental results. However, it is felt that the needs for evaluated data other than (n, γ) on the fission products are not met by the existing evaluated data libraries and, in addition, data on fission product decay and resonance parameter sets are not always available in the evaluated data files. Accompanying its reply to our Circular Letter, Sweden submitted a preliminary list of requests for data evaluations which is given in Annex III.

In the case of India, the ENDF/B and KEDAK libraries are available, however, the processing computer codes are yet to be commissioned. Once this is accomplished, the libraries and codes will be used extensively. Their needs for evaluated neutron data arise from their reactor programme in which special materials have been used. For example, the Indian Pulsed Fast Reactor uses copper as a reflector and their Fast Breeder Test Reactor (40 MWt) uses a thorium blanket and nickel reflector. They therefore require evaluated data for Cu, Th, Ni and U-233. In contrast, Israel, Finland and Greece felt that the existing evaluated data libraries were adequate to satisfy the needs of their users, whilst Denmark had a need for evaluated data at some elevated temperatures, especially for the fissile nuclei, and the Netherlands considered that the existing evaluated data sets were more than sufficient to satisfy their needs, except in the case of the fission products. South Africa stated that its evaluated data requirements were small and therefore reasonably well met by the existing data libraries, and Belgium considered that its limited needs for evaluated data were fulfilled to a large extent by the existing libraries, except in the case of tantalum for which it was felt that a revision of the existing data was required.

There are some needs for evaluated neutron data at the Federal Institute for Reactor Research (Switzerland). The ENDF/B library, which the Institute has largely satisfies their present needs, however, their additional needs for evaluated data refer to data on He-4, Be (n,2n), B-11, Si and Ca. At present, this Institute only uses data libraries such as GGC-3, FD-2, FD-4, Mural-Fresco and Thermos since their Mc^2

programmes are not as yet ready to manipulate the evaluated data. They experience some restrictions due to the limited memory of their computers (CDC-6500), however, they expect that even after completion of their own Mc^2 version programmes the use of effective group cross-section sets will in most cases be sufficient. Though their present needs are in the main satisfied, they expect an increased interest in evaluated data in the future. Australia has access to the ENDF/B and UKNDL libraries and their limited experience to-date with these libraries has indicated that the required information can be provided, though the adequacy and accuracy of the data are often in doubt. The complete contents of KEDAK and some files from the UKNDL are available in Hungary, and in his reply Dr. P. Vertes (Hungary) noted that the assortment of the nuclei in the KEDAK and UKNDL libraries was not satisfactory. In addition, they needed a higher upper energy boundary in order to meet the requirements of shielding calculations and activation analysis. In Norway the need for evaluated data for their reactor calculation code systems is felt very strongly and this will be even more so in the future, however, the full utilization of the existing data libraries is hampered by the lack of suitable codes for processing the data libraries. Turkey felt that their existing data libraries, which contained a very limited amount of rare element total neutron cross section calculational codes and experimental data, satisfied their needs for the time being, however, more up-to-date neutron cross section data for the materials present in thermal reactors are needed.

Finally, in the case of Argentina, there is an interest to use evaluated neutron data to generate multigroup cross sections for reactor and neutronics calculations. This interest has emerged due to the gradual shift in their interests towards fast reactor physics. They are at present using the multigroup cross-section set from Karlsruhe, but, in the future, they wish to generate their own multigroup cross sections. This desire however does have its associated problems since the computers needed to handle the service programmes and the multigroup generation programmes must be sufficiently large and secondly, the computational effort required to make a system such as this operational must also be rather sizeable. In conclusion, Dr. G.H. Ricabarra (Argentina) pointed out that their main interest is in using the evaluated data produced by the exchange through the 4-Centres rather than in evaluation per se.

though this did not exclude the possibility that some limited evaluation work may be done in the future in Argentina.

V. Conclusions.

This review has aimed at assessing the evaluation activities and the needs for evaluated neutron data for a broad spectrum of Member States at different levels of nuclear development. However, despite this wide scope there are four important points which have clearly emerged. In the first place, for most of those States with a fully integrated neutron nuclear data cycle and which are particularly active in performing evaluations, the establishment of the Neutron Nuclear Data Evaluation Newsletter (NNDEN) by the E.A.N.D.C. - E.A.C.R.P. Joint Sub-Committee on Nuclear Data Evaluation, has led to some significant progress in achieving, at least, a partial degree of multi-national cooperation amongst the contributing States.

Secondly, considerable progress is being and has been made in overcoming the major problems of translating from the format of one evaluated data library to another. Indeed, at present, conversion programmes either exist or are being developed for most of the major libraries. Thirdly, in the replies from several States special attention was given to the question of the inadequacy of the existing evaluated data libraries both with regard to the number of materials contained in the libraries (i.e. the quantity of data), and also the insufficient accuracy (i.e. the quality) of the data contained therein.

Finally, for most of those States not possessing a fully integrated neutron nuclear data cycle, it is evident that their efforts in the field of performing evaluations will necessarily be focused on small specialized areas where it is felt that significant contributions can be made. In addition, in relation to their needs for evaluated data, the immediate problem for these States is not really that of being able to gain access to evaluated neutron data libraries since, at least, one such complete library is already available through the Agency. However, their real problems in dealing with evaluated data are related to the limitations they experience in not being able to automatically handle the large evaluated data files and their accompanying editing and processing programmes, because their computer facilities must not only be sufficiently large but also the computational effort required, for example, to generate

their own multi-group cross-section sets, is considerable. It is important to recall that these States include not only the developing countries, but also some of the economically developed States. This therefore implies that in considering the needs and interests of these States attention should also be given to the possibility of assisting them in gaining access to well updated sets of multi-group cross sections.

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Table I

Neutron Data Evaluation Work in Progress(I) and Planned(II) to be Started During the Next 6 Months

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories)
$H^{(I)}$	$\sigma_{n,T}$	0.7 Mev - 15 Mev	Fed.Rep.Germany	Meyer (G.f.K.)
* $H^{(I)}$	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart, La Bauw, Young (L.A.S.L.)
$D^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart (L.A.S.L.)
$T^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart (L.A.S.L.)
$He\text{-}3^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart (L.A.S.L.)
$He\text{-}4^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart (L.A.S.L.)
$Li\text{-}6^{(I)}$	$\sigma_{n,\alpha}$	10 Kev - 500 Kev	France	Mezza, Ribon (C.E.N./Saclay) and Fort (C.E.N./Cadarache)
$Li\text{-}6^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart (L.A.S.L.)
$Li\text{-}6^{(I)}$	All Major Reaction Types, especially $\sigma_{n,n}$, $\sigma_{n,t}$	Thermal - 5 Mev	U.K.	Uttley and Sowerby (A.E.R.E.)
$Li\text{-}7^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Stewart (L.A.S.L.)
* $Be^{(I)}$	All Major Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Perkins and Howerton (L.R.L.)
$C^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Perey (O.R.N.L.)
$C^{(II)}$	Thermal Scattering Law, effect of anisotropy of graphite crystals		U.K.	Butland (A.E.E.W.)

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories)
* $N^{(I)}$	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Young and Foster (L.A.S.L.)
$O^{(I)}$	All Reaction Types	Thermal - 15 Mev	U.S.S.R.	
* $O^{(I)}$	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Young and Foster (L.A.S.L.)
$Na^{(I)}$	All Reaction Types	Thermal - 15 Mev	U.S.S.R.	
* $Na^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Pitterle (W.A.R.D.) and Perey (O.R.N.L.)
$Na^{(II)}$	$\sigma_{n,T}$	Above threshold of inelastic scattering process - 15 Mev	Fed.Rep.Germany	Meyer (G.f.K.)
$Na^{(I)}$	$\sigma_{n,T}$, $\sigma_{n,n'}$, $\sigma_{n,n'}$	8 - 14 Mev	Italy	Benzi et al (C.D.C.)
* $Mg^{(II)}$	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Howerton (L.L.L.)
* Al	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Young and Foster (L.A.S.L.)
$Si^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Kinsey (B.N.L.)
$S^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Drake (B.N.L.)
$S-32^{(I)}$	$\sigma_{n,n}$, $\sigma_{n,n'}$, $\sigma_{n,p}$	1 Mev - 10 Mev	Romania	(I.F.A.)
$Ca^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Perey (O.R.N.L.)
$Cr^{(II)}$	$\sigma_{n,T}$	Above threshold of inelastic scattering process - 15 Mev	Fed.Rep.Germany	Meyer (G.f.K.)
$Cr^{(II)}$	$\sigma_{n,\gamma}$	100 eV - 1 Mev	France	Le Coq (C.E.N./Saclay)

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories)
$Cr^{(I)}$	$\sigma_{n,n}$, $\sigma_{n,T}$	8 Mev - 15 Mev	Romania	(I.F.A.)
$Cr^{(I)}$	$\sigma_{n,n'}$ $\sigma_{n,\gamma}$	Resonance Region	U.K.	Moxon (A.E.R.E.)
* $Fe^{(I)}$	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Young and Foster (L.A.S.L.)
$Fe^{(II)}$	$\sigma_{n,T}$	Above threshold of inelastic scattering process - 15 Mev	Fed.Rep.Germany	Meyer (G.f.K.)
$Fe^{(II)}$	$\sigma_{n,\gamma}$	100 eV - 1 Mev	France	Le Coq (C.E.N., Saclay)
$Fe^{(I)}$	$\sigma_{n,n}$, $\sigma_{n,T}$	8 Mev - 15 Mev	Romania	(I.F.A.)
$Fe^{(I)}$	All Reaction Types	Thermal - 15 Mev	U.S.S.R.	
$Co^{(II)}$	$\sigma_{n,\gamma}$	1 Kev - 10 Mev	Romania	(I.F.A.)
$Ni^{(II)}$	$\sigma_{n,\gamma}$	100 eV - 1 Mev	France	Le Coq (C.E.N., Saclay)
$Ni^{(II)}$	$\sigma_{n,T}$	Above threshold of inelastic scattering process - 15 Mev	Fed.Rep.Germany	Meyer (G.f.K.)
$Ni\text{-}60^{(I)}$	$\sigma_{n,n'}$, $\sigma_{n,n'}$, $\sigma_{n,p}$	1 Mev - 10 Mev	Romania	(I.F.A.)
$As\text{-}75^{(II)}$	$\sigma_{n,\gamma}$	1 Kev - 10 Mev	Romania	(I.F.A.)

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories)
$Mo^{(II)}$	$\sigma_{n,T}$	Above threshold of inelastic scattering process - 15 Mev	Fed.Rep.Germany	Meyer (G.f.K.)
$Mo^{(I)}$	$\sigma_{n,n'}$, $\sigma_{n,n'}$, $\sigma_{n,\alpha}$	Fast Region	U.K.	Douglas (A.W.R.E.)
$Ag\text{-}107^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Bhat (B.N.L.)
$Ag\text{-}109^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Bhat (B.N.L.)
$Xe\text{-}135^{(II)}$	$\sigma_{n,\gamma}$	200 eV - Mev region	Italy	Benzi et al (C.D.C.)
$Cs\text{-}133^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Bhat (B.N.L.)
Natural $Gd^{(I)}$ isotopes	All Reaction Types	1 Kev - 10 Mev	Italy	Benzi et al (C.D.C.)
$Ta^{(II)}$	$\sigma_{n,\gamma}$	1 Kev - 10 Mev	Romania	(I.F.A.)
$W^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Devaney (L.A.S.L.)
$W^{(II)}$	$\sigma_{n,\gamma}$	1 Kev - 10 Mev	Romania	(I.F.A.)
$W\text{-}182^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Alter (A.I.)
$W\text{-}183^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Alter (A.I.)
$W\text{-}184^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Alter (A.I.)
$W\text{-}186^{(I)}$	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Alter (A.I.)
Au-197	$\sigma_{n,\gamma}$	Thermal - 10 Mev	U.S.S.R.	

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories)
Pb(I)	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Perey (O.R.N.L.)
Pa-233(II)	$\sigma_{n,n'}$	6 Kev - 500 Kev	Japan	Ohta (Kyushu Univ.)
U-235(II)	All Reaction Types	Thermal - 15 Mev	Japan	Nishimura, Igarashi, Nakasima (J.A.E.R.I.), Matsunobu (Sumitomo), Iijima (N.A.I.G. Kanda (Kyushu Univ.) et al
U-235(I)	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Smith (I.N.C.), Pitterle (W.A.R.D.) and Alter (A.I.)
U-235(I)	$\sigma_{n,T}$	200 eV - 15 Mev	Fed.Rep.Germany	Hinkelmann (G.f.K.)
U-235(II)	α	eV range up to 15 Mev	Fed.Rep.Germany	Hinkelmann (G.f.K.)
U-235(I)	$\sigma_{n,f}$	Thermal - 15 Mev	France	Le Coq and Ribon (C.E.N./Saclay)
U-235(I)	Resonance Parameters	$<$ 100 eV	France	Le Coq and Ribon (C.E.N./Saclay)
U-235(I)	All Reaction Types	Thermal - 15 Mev	U.S.S.R.	
U-238(II)	All Reaction Types	Thermal - 15 Mev	Japan	Nishimura, Igarashi and Nakasima (J.A.E.R.I.), Matsunobu (Sumitomo), Iijima (N.A.I.G Kanda (Kyushu Univ.) et al
U-238(II)	$\sigma_{n',T}$	Kev - Mev region	Fed.Rep.Germany	Hinkelmann (G.f.K.)
U-238(II)	$\sigma_{n,T}$	Kev - Mev region	Italy	Zuffi et al (C.D.C.)
U-238(I)	All Reaction Types	Thermal - 15 Mev	U.S.S.R.	

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories
U-238(I)	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Pitterle (W.A.R.D.)
Np-239(II)	$\sigma_{n,n'}$	30 Kev - 1 Mev	Japan	Ohta (Kyushu Univ.)
Pu-238(I)	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	(L.A.S.L.)
Pu-239(I)	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	Smith (I.N.C.), Pitterle (W.A.R.D.) and Hutchins (A.I.)
* Pu-239	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Young and Foster (L.A.S.L.)
Pu-239(I)	$\sigma_{n,f}$ and $\sigma_{n,\gamma}$	1 eV - 100 eV	Australia	Cook and Bertram (A.A.E.C.)
Pu-239(II)	All Reaction Types	Thermal - 15 Mev	Japan	Nishimura, Igarashi and Nakasima (J.A.E.R.I.), Matsunobu (Sumitomo), Iijima (N.A.I.G.) Kanda (Kyushu Univ.)
Pu-239(I)	All Reaction Types	Thermal - 15 Mev	U.S.S.R.	
Pu-239(II)	Parametrization of neutron cross sections	Thermal - 15 Mev	Bulgaria	Ianeva (B.A.S.)
Pu-240(I)	All Reaction Types	Thermal - 15 Mev	Israel	Yiftah and Caner (S.N.R.C.)
* Pu-240	All Reaction Types	10^{-5} eV - 20 Mev	U.S.A.	Young and Foster (L.A.S.L.)
Pu-241(I)	All Reaction Types	Thermal - 15 Mev	Israel	Yiftah and Caner (S.N.R.C.)
Pu-241(II)	All Reaction Types	Thermal - 15 Mev	Japan	Nishimura, Igarashi and Nakasima (J.A.E.R.I.), Matsunobu (Sumitomo), Iijima (N.A.I.G.) Kanda (Kyushu Univ.) et al

Nuclide	Cross Section Type	Energy Range	Member State	Evaluators' Names (Laboratories)
Pu-242(I)	All Reaction Types	Thermal - 15 Mev	Israel	Yiftah and Caner (S.N.R.C.)
Fission Products(I)	$\sigma_{n,\gamma}$, $\sigma_{n,n'}$, $\sigma_{n,2n}$	1 Kev - 10 Mev	Italy	Benzi et al (C.D.C.)
Fission Products(I)	$\sigma_{n,\gamma}$	1 eV - 10 Mev	Netherlands	Lautenbach (R.C.N.)
Fission Products(II)	$\sigma_{n,\gamma}$, $\sigma_{n,n'}$, etc.	0.1 Kev - 15 Mev	Japan	Iijima (N.A.I.G.)
Fission Products(I)	Major Reaction Types	0.001 eV - 15 Mev	Australia	Cook and Clayton (A.A.E.C.)
Fission Products(I)	All Major Reaction Types	Thermal - 15 Mev	U.S.A.	(B.N.L.), (B & W) and (W.A.D.C.O.
Many Nuclides(I)	Charged particle emission - systematic analysis of experimental data available	Mev region	Italy	Reffo et al (C.D.C.)
Many(I)	Capture γ-rays	Kev Neutron capture	Australia	Bird, Allen and Kenny (A.A.E.C.)
Nearly All Stable Nucleii(I)	$\sigma_{n,2n}$ Recommendation of most probable values and systematics of (n,2n) cross sections based on N-Z dependence	14 Mev	Hungary	Bödy and Csikai (I.E.P.)
Nearly All Stable Nucleii(I)	$\sigma_{n,\Gamma}$ Investigation of fine and gross structions	13 - 15 Mev	Hungary	Angeli and Csikai (I.E.P.)

* includes γ-ray production cross sections.

List of Laboratory Abbreviations Used in Table I.

State	Laboratory Code	Laboratory
Australia	A.A.E.C.	Australian Atomic Energy Commission Research Establishment
Bulgaria	B.A.S.	Bulgarian Academy of Sciences - Institute of Physics and Nuclear Research Centre
Fed. Rep. Germ.	G.f.K.	Gesellschaft für Kernforschung m.b.H., Institut für Neutronenphysik and Reaktortechnik
France	C.E.N/	Centre d'Etudes Nucléaires/
Hungary	I.E.P.	Institute of Experimental Physics, Kossuth University
Israel	S.N.R.C.	Soreq Nuclear Research Centre
Italy	C.D.C.	Centro di Calcolo
Japan	J.A.E.R.I.	Japan Atomic Energy Research Institute
	N.A.I.G.	Nippon Atomic Industry Group Co., Ltd.
	M.A.P.I.	Mitsubishi Atomic Power Industries, Inc.
	Sumitomo	Sumitomo Atomic Energy Ltd.
Netherlands	R.C.N.	Stichting Reactor Centrum Nederland
Romania	I.F.A.	Institute of Atomic Physics
U.K.	A.E.R.E.	Atomic Energy Research Establishment, Harwell
	A.E.E.W.	Atomic Energy Establishment, Winfrith
	A.W.R.E.	Atomic Weapons Research Establishment, Aldermaston
U.S.A.	L.A.S.L.	Los Alamos Scientific Laboratory
	L.L.L.	Lawrence Livermore Laboratory
	O.R.N.L.	Oak Ridge National Laboratory
	W.A.R.D.	Westinghouse Advanced Reactors Division

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U.S.A. (cont'd)	B.N.L.	Brookhaven National Laboratory
	B & W	Babcock and Wilcox Inc.
	W.A.D.C.O.	
	A.I.	Atomics International Inc.
	I.N.C.	Idaho Nuclear Corporation

Table II

The Computer Facilities Abailable for Performing Evaluations and for Handling Evaluated Data Libraries

Member State	Institute(s)	Computer Facilities and Systems
Argentina	1. Centro Atomico - Bariloche 2. Comision Nacional de Energia Atomica - Buenos Aires.	A computer with 32 K total memory. IBM-360/65, total memory 160 K.
Australia	1. Australian Atomic Energy Commission.	IBM-360/50I, with disk packs, tape drivers, etc.
Belgium	1. Centre d'Etude de l'Energie Nucléaire, Mol. 2. Liège.	IBM-360/44 IBM-360/65
Bulgaria	Bulgarian Academy of Sciences, Institute of Physics and Nuclear Research Centre	ICL and Gier computers
Denmark	Atomic Energy Commission, Research Establishment Risö	IBM-360/65, IBM-7094, Burroughs - 6500
France	Centre d'Etudes Nucléaires de Saclay	IBM-360/91 and CDC-6600
Fed. Rep. Germany	Kernforschungszentrum Karlsruhe	IBM-360-65/85
Greece	Nuclear Research Centre, Democritos	CDC-3300
Hungary	1. Institute of Experimental Physics, Kossuth University 2. Hungarian Academy of Sciences. Central Research Institute for Physics	ODRA - 1204 and ODRA - 1013 ICL - 1905, 32 K memory.
India	Bhabha Atomic Research Centre	CDC-3600, 32 K memory

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Israel	1. Soreq Nuclear Research Centre 2. Weizman Institute, Rehovot with terminal at Soreq 3. Israel Institute of Technology, Technion	IBM-360/65 and Philco - 212 IBM-370/165 IBM-370/165
Italy	Comitato Nazionale per l'Energia Nucleare - Centro di Calcolo	IBM-7094/7040 coupled system, 32 K memory. IBM-1401, IBM-360/75. IBM-1627 Data Plotter and IBM-2250/1 Display Unit
Japan	Japan Atomic Energy Research Institute, Tokai Research Establishment	CDC-6600, IBM-360/75 FACOM-230/60, etc.
Netherlands	1. Reactor Centrum Nederland 2. University of Delft	Electrologica-X8. After July 1972 a CDC-6600. IBM-360/65
Norway	Institutt for Atomenergi, Kjeller	CDC-3600. Will be replaced by a new machine in one year
Romania	Institute of Atomic Physics	Access to IBM-360/40 and Elliott-4100
Sweden	1. Research Institute of the Swedish National Defense 2. AB Atomenergi-Studsvik	IBM-360/75 Access to a CDC-6600 with a terminal in Studsvik
Switzerland	Institut Federal de Recherches en Matière de Réacteurs, Würenlingen	CDC-6500
Turkey	Istanbul Technical University	IBM-1620
U.S.A.	1. Los Alamos Scientific Laboratory 2. Lawrence Radiation Laboratory 3. Oak Ridge National Laboratory 4. Brookhaven National Laboratory 5. Atomics International 6. Westinghouse Advanced Reactors Div. 7. Babcock and Wilcos Co. 8. W.A.D.C.O. 9. I.N.C.	The computer facilities are very varied. Two systems are used for the evaluation of cross sections: 1. SCORE-II - An Interactive Neutron Evaluation System, by C.C. Dunford et al, AI-AEO-12757 (1969) 2. ACSAP - The Automated Cross Section Analysis Program, by N.H. Marshall et al. Third Conf. on Neutron Cross Sections and Technology, Knoxville (1971)

U.K.	1. Aldermaston Weapons Research Establishment,	IBM-360/75, an IBM-2250 CRT console is linked to the computer. A Ferranti Atlas computer is also available and is used sometimes by evaluators to generate input for a CRT plotter.
–	2. Atomic Energy Research Establishment.	IBM - 360/75; a Calcom CRT plotter is available.
	3. Atomic Energy Establishment, Winfrith.	KDF-9 and ICL-4/70; an IBM-360/ is used for tape copying /30 and mode conversions and to provide a link to the Harwell computer.
U.S.S.R.	1. Nuclear Data Centre, Obninsk,	M-222 computor to be used in conunction with a Benson graph plotter.
	2. Computer Centre, Institute of Physics and Power Engineering, Obninsk,	M-220 computer
	3. Institute of Theoretical and Experimental Physics (Moscow),	
	4. The Institute of Nuclear Research of the Ukrainian SSR Academy of Sciences (Kiev),	The computers at the other Institutes include "Mir", "Nairi" etc.
	5. Institute of Nuclear Energy of the Byelorussian SSR Academy of Sciences (Minsk).	

Table III

Evaluated Neutron Data Libraries Available in Member States

Libraries developed in a specific Member State are denoted by an asterisk(*)

Member State	Evaluated Data Library Used
Argentina	KEDAK and certain files of the UKNDL
Australia	UKNDL and ENDF/B
Belgium	UKNDL, KEDAK and ENDF/B
Brazil	Certain files of the UKNDL
Bulgaria	None at present
Czechoslovakia	Certain files of the UKNDL
Denmark	UKNDL, RESAB(*) - A resonance parameter library and FIPO(*) - A 10 group fission product cross section library
Finland	KEDAK and certain files of the UKNDL
France	UKNDL, ENDF/B and KEDAK
Fed.Rep.Germany	KEDAK(*) and ENDF/B. The format of KEDAK is given in the report KFK-880
Greece	None at present
Hungary	KEDAK and certain files from the UKNDL
India	KEDAK, ENDF/B and certain files of the UKNDL
Israel	UKNDL, KEDAK and ENDF/B
Italy	ENDF/B, KEDAK and UKNDL
Japan	ENDF/B, KEDAK, UKNDL, ENDF/A (old)
Korea, Rep. of	KEDAK and certain files of the UKNDL
Netherlands	UKNDL, ENDF/B and KEDAK will all be available at Delft in the near future
Norway	UKNDL and ENDF/B are to be acquired

Member State	Evaluated Data Library Used
Romania	KEDAK and certain files of UKNDL
South Africa	KEDAK and certain files of the UKNDL
Sweden	UKNDL and ENDF/B. The SPENG(*) library (in free format) which contains effective group cross sections in the 4 eV to about 30 Kev region and point cross sections elsewhere from thermal to about 15-18 Mev. A description of the "element data" is given in the AB Atomenergi Internal Report, AE-RFN-279 (1967) describing the SPENG(*) library - (see also Annex II of this Review)
Switzerland	ENDF/B
Turkey	None at present
U.S.S.R.	The complete KEDAK library is available and certain files from the UKNDL. Work is in progress on establishing a USSR Evaluated Neutron Data Library(*) based on a format developed in the USSR and described at the Soviet-Belgian-Dutch Symposium held at Melekess (U.S.S.R.) in February 1970. (See Reports INDC(FR)-2/L by P. Ribon and INDC(CCP)-13/L by V.E. Kolessov and M.N. Nikolaev (1971).
U.K.	UKNDL(*) ENDF/B and GENEX(*). The library GENEX contains resonance cross section data in great detail (120,000 energy points) from 0.4 eV to 25 Kev for a few fertile and fissile materials U-235, U-238, Pu-239, Pu-240 and Pu-241. The data are in binary format, see Report AEEW-R-622 (1968). The format of the UKNDL is given in the Report AWRE-O-70/63 by K. Parker.
U.S.A.	ENDF/A(*), ENDF/B(*), KEDAK, UKNDL. The ENDF format is described in the Report ENDF-102 (BNL-50274). LLL(*) the LLL Format is described in UCRL-50400, Vol. IV.
Yugoslavia	KEDAK and certain files of the UKNDL

Table IV

Programmes and Codes for Evaluated Data Handling

Codes developed in a specific Member State are denoted by an asterisk(*)

Member State	Programmes and Codes Available
Australia	The normal ENDF/B programmes for editing, checking and updating. Small local programmes(*) for various minor features.
Belgium	No special programmes for evaluated data handling have been developed at the C.E.N./Mol, but several programmes developed elsewhere are available.
Denmark	SIGMA(*) - an Algol version of GALAXY for editing and updating group cross section on the basis of new UKNDL versions.
Fed.Rep.Germany	1. For retrieval of KEDAK data - NDF(*) programme package. 2. KEDABE(*) - Updating mutually dependent cross section types consistently for the KEDAK library. 3. SGIPAR(*) - Printing inelastic excitation cross sections from KEDAK. 4. SELDIF(*) - Printing of the differential elastic scattering cross sections. 5. A programme(*) for printing all microscopic data for a given material in a given energy range. 6. KEMA(*) - for updating the KEDAK library; e.g. for deletion, insertion, change of records. 7. SELPLO(*) - A programme for plotting the elastic scattering angular distributions.
France	A programme(*) to verify the UKNDL format.
Hungary	1. PRODGROUP(*) - A programme for the production of multi-group reactor constants from the evaluated nuclear data available from the IAEA, Report KFKI-71-4. 2. A MUFT(*) type 40 group constant library, Report INDC (HUN)-4/G.
India	The codes CRECT, CHECKER, RIGEL, DICTION and SLAVE (see U.S.A. for descriptions).
Israel	1. CHCK(*) - A code for checking the ENDF/B, UKNDL and KEDAK libraries. 2. CRECT (see U.S.A. for description). 3. PLOT - Graphical representation of data for ENDF/B, KEDAK, and UKNDL libraries.

Member State	Programmes and Codes Available
Italy	1. PRECOD(*); 2000; 3000; CODUK(*) - An automated chain of codes for generating a UK Nuclear Data File. 2. FILE 2(*) - A programme for producing an interpolated list of ENDF/B-II resonance data. 3. CHECKER, NDF PRINT, IDA(UKNDL). 4. The codes described in the report ENDF-110.
Japan	Data-processing codes(*) are presently being prepared and will be completed at the end of March 1972.
Netherlands	The processing codes developed at the Institutes in other Member States.
Norway	Only codes for listing the contents of the UKNDL, but no codes for processing the contents of the UKNDL.
Sweden	1. All ENDF/B processing codes and programmes are available, however only DAMMET (see U.S.A. for description) has been used. 2. For processing the SPENG library a programme DSPENG(*) is used.
U.S.A.	The following data handling codes are used and documented in the report ENDF-110 (to be issued as a BNL report):- 1. CRECT(*) - Corrects data on an ENDF/B BCD card image tape. 2. CHECKER(*) - Checks structure, formats and consistency of data on an ENDF/B BCD card image tape. 3. RIGEL(*) - Retrieves, merges, changes mode or arrangement of the data on ENDF/B tapes. This code replaces DAMMET. 4. PLOTFB(*) - Interprets data from BCD or Binary ENDF/B tapes and produces edited listings and/or Calcomp plots. 5. LISTFC(*) - Produces interpreted listings of data from an ENDF/B, BCD card image tape. 6. DICTION(*) - Produces a new section dictionary for an ENDF/B BCD card image tape. 7. SLAVE-3(*) - Retrieval subroutines and selected averages of ENDF/B File 3 data. 8. CLYDE(*) - Documented in UCRL-50400 Vol. V. Processes data from LLL file to group constants and transfer matrices for unlimited number of groups and arbitrary Pl order.

Member State	Programmes and Codes Available
U.S.S.R.	Work is in progress on programmes both for establishing and maintaining the USSR Evaluated Nuclear Data Library and for using the data in the Library. At present, the following programmes are in use:- 1. A programme(*) for printing out collections of information from the evaluated nuclear data library in the form required by the user (e.g. several tabular arrangements for presenting the information). 2. POSOSHOK(*) - A programme for checking the information presented in the format of the USSR Evaluated Nuclear Data Library. 3. A programme(*) for correcting and making additions to the information contained in the USSR Evaluated Nuclear Data Library. 4. A number of other programmes(*) for various purposes.
U.K.	1. LCHECK(*) - Written in Egtran-2(1) language for the KDF-9 Computer. Reads cards to tape with elementary sequential check. 2. CHECK-1(*) - Written in Fortran-4(2) for the IBM-360/75 computer. Checks format and arthimetical consistency of data files. 3. CHECK-2(*) - Written in Fortran-2 for the KDF-9 computer. 4. AMEND(*), JACKDAW(*), GRAFT-3(*) - Written in Egtran-2(1) for the KDF-9 computer. For amending and modifying data files in various ways. 5. EDIT(*) - Written in Egtran-2(1) for the KDF-9 computer. For merging files from various tapes to form a data library. 6. MINIGAL(*) - Written in Egtran-2(1) for the KDF-9 computer. Computes resonance integrals and fission-spectrum averaged cross sections from a data file. 7. GROD(*) - Written in Fortran-4 for the IBM-360/75 computer. Prepares tapes for graphical representation of data using a CRT plotter. 8. PANDIT(*) - Written in Fortran-4(2) for the IBM-360/75 computer. For adjusting UKNDL data files from calculated adjustments to group cross sections(3). 9. GALAXY(*) - Written in Egtran-2(1) for the KDF-9 computer and in Fortran-4(2) for the IBM-360/75 computer. Principal users' programme for computing multi-group cross sections from the UKNDL.

(1). Egtran-2 is a dialect of Fortran-2 developed for the KDF-9 computers.

(2). Conversion of these programmes to Fortran-4 is in progress.

(3). It should be emphasized that adjustments of this kind have not been made to any of the basic data files in the UKNDL.

Table V

Computer Programmes and Codes for the Analysis and Calculation of Cross Sections

Codes developed in a specific Member State are denoted by an asterisk(*)

Member State	Code	Brief Description of Code
Australia	1. COMPOST	Optical Model Code based on Perey and Buck.
	2. GUNYA	Cross-section generation codes for thermal and resolved resonance region. Uses single-level Breit-Wigner formulation and treats unresolved resonances up to d-waves.
	3. RESP and GENEX	The UKAEA cross section generation codes - Vogt multilevel formulation.
	4. CODILLI	Adler based fitting and cross section generation code.
	5. MULFT(*)	Similar to Adler's but faster than CODILLI, based on theory by J. Cook (A.A.E.C.).
Belgium	SHAPTRA(*)	Total cross-section analysis in terms of single level Breit-Wigner parameters - contains several options and improvements over earlier programmes of this kind. A scattering cross-section programme is also being developed but not yet operational
France	1. _____	Programmes(*) to analyze resonances.
	2. FISINCA, NEARREX, SAUDEX, etc.	Programmes based on the statistical model.
	3. MAGALI, GENOA, ABACUS, etc.	Programmes based on the spherical optical model.
	4. ECIS70, JUPITOR	Programmes based on the deformed optical model.
Fed.Rep.Germany	1. NEARREX	Calculates radiative capture, fission, compound elastic and inelastic neutron cross sections and proton induced average cross sections using Hauser-Feshbach theory.
	2. _____	Optical model code based on Perey and Buck.

Member State	Code	Brief Description of Code
Hungary	1. PRODGROUP(*)	Programme for production of multigroup reactor constants from the evaluated nuclear data available from the IAEA. Report KFKI-71-4.
	2. _____	A KUFT type(*) 40-group constant library. Report INDC(HUN)-4/G
India	1. CAREFREE(*)	Code for calculation of point cross sections as a function of temperature from single level Breit-Wigner formulae.
	2. COMPLEX	Calculates neutron cross sections of fissionable elements for 25 interfering resonances per spin state using complex poles of the collision matrix.
	3. LEXA	Calculates S-wave resonance cross sections for fissionable elements with a given set of R-matrix parameters.
	4. INTERFERE	Calculations cross sections and complex partial widths for interfering resonances from a given set of R-matrix parameters.
	5. MLBW	Calculates cross sections for mixtures of non-fissile isotopes of an element from resonance parameters using multi-level Breit-Wigner formulation.
	6. IRCLMIKP(*)	Code to evaluate S-wave neutron resonance cross sections for the fissionable elements from a given set of R-matrix parameters.
	7. NEARREX, MC^2, ABACUS, TEMPO	
Israel	1. ABACUS-2/NEARREX	optical model and statistical theory.
	2. COMBCO	Resonance cross sections.
	3. NANICK	Multigroup cross section set from ENDF/B libraries.
Italy	1. For Radiative Neutron Capture	
	A. FISPRO-II(*)	Compound and estimate for direct and collective.
	B. SAUD(*)	Compound; l = 0,1.
	C. DIRCO(*)	Dipole direct and collective.
	D. KISS(*)	Quadrupole direct.
	E. SPEC	γ-ray spectra cross-compound capture.

Member State	Code	Brief Description of Code
Italy (ctd.)	2. Non-elastic	
	A. SASSI(*)	Hanser-Feshbach (n,n') with spherical optical model penetrabilities.
	B. EXODUS(*)	Same as SASSI(*) for unresolved inelastic scattering cross sections.
	C. NEFASS(*)	Evaporation model.
	D. HARE(*)	Evaporation model for (n,a,b,c) neutrons
	E. NEARREX, JANE, ABACUS	
	3. Optical Model	
	A. SKOC(*)	Spherical optical model.
	B. DANC(*)	Rotational even-even nuclei
	C. ADAPE(*)	Deformed nuclei; adiabatic.
	D. EMOC(*)	Even-even nuclei with microscopic description of target states.
	E. JUPITOR, 2-PIUS	
	4. Photoreactions	
	A. SURF(*)	Coupled channel - one particle-one hole continuum approximation.
	5. Miscellaneous	
	A. LILABNER(*)	Level density parameter from Dobs.
	B. AVERAGE, NLBW, SLP, SIGPLOT	
Japan	1. ELIESE-I & II	Eliese-II (Report JAERI-1169,1968) Optical model, Hauser-Feshbach and Moldauer theories are used in Eliese.
	2. JUPITOR-I	JAERI-Memo-3633(1969) - inelastic scattering cross section on basis of coupled-channel method.
	3. MOLDOR	
	4. MCROSS	
	5. TOTAL	Surveys systematics of optical potential parameters.
	6. RACY	JAERI-Memo-3300(1968) calculates (n,γ) cross section on statistical and direct interaction models.
	7. STEVE, etc.	
Romania	Programme for a local optical model with parameter selecting. Programme based on Hauser-Feshbach-Moldauer calculations. Programme for calculating elastic cross sections being developed. Programme for calculation local parameters on basis of multi-level R-matrix theory.	

Member State	Code	Brief Description of Code
Sweden	1. FLANGE-II	Code to process thermal neutron scattering data from the ENDF/B library.
	2. ETOX	Code to calculate group constants for nuclear reactor calculations. Report BNWL-1002.
	3. ABACUS/NEARREX	Elastic, inelastic cross sections and angular distribution calculations.
Sweden (ctd.)	4. _____	A programme for optical model calculations of non-spherical nucleii by P. Fabbry and L. Zuffi.
	5. DORIX-STENG(*)	Computation of resonance screened cross sections and neutron spectrum. Report AE-334 (1968) by H. Häggblom.
	6. SUM-CC(x)	A semi-direct radiative capture code by J. Eriksson.
U.S.A.	1. ABACUS-II(*)	Optical model-spherical potential.
	2. JUPITOR,(*) 2-PLUS(*)	Optical model-coupled channel.
	3. NEARREX(*), COMNUC(*), FISPRO-II	Compound nucleus.
		The above are representative of the codes used in U.S.A. laboratories.
U.S.S.R.	1. _____	Programmes(x) for calculating cross sections on the basis of statistical theory and the optical model.
	2. _____	Programmes(x) for calculating cross sections in the allowed-resonance region on the basis of the S-matrix and R-matrix formalisms.
	3. _____	A programme(*) for calculating the mean structural characteristics of cross sections in the forbidden-resonance region, etc.
U.K.	1. LEAP(*)	Written in Fortran-4 for ICL-4/70 computor. Calculates thermal scattering law from phonon frequency function in incoherent model.
	2. SLAB(*)	
	3. TOR(*)	
	4. PIXSE(*)	Written in Egtran-2(1) for KDF-9 computer, and in Fortran-4 for ICL-4/70 computer.
	5. SOLON(*)	Written in Fortran-4 for ICL-4/70 computor
	6. GLEN(*)	
		PIXSE, SOION and GLEN calculate inelastic cross sections from scattering law.
	7. HEXCOH(*)	Written in Egtran-2(1) for the KDF-9 computor. Calculates coherent elastic scattering of monatomic hexagonal crystals.

Member State	Code	Brief Description of Code
	8. SIGAR(*)	Written in Egtran-2(1) for the KDF-9 computer. Calculates $\sigma_{n,T}$, $\sigma_{n,n}$, $\sigma_{n,\gamma}$ in multilevel Breit-Wigner formalism for l = 0 to 5. Doppler broadened output in UKNDL format.
U.K. (ctd.)	9. REMO(*)	Written in Egtran-2(1) for the KDF-9 computer. Calculates $\sigma_{n,T}$, $\sigma_{n,n}$, $\sigma_{n,\gamma}$, $\sigma_{n,f}$ by Reich-Moore method, for l = 0 only. Provides input to TEMPO.
	10. TEMPO(*)	Written in Egtran-2(1) for the KDF-9 computer. Doppler broadening of arbitrary cross sections with output in UKNDL format.
	11. MLCSC(*)	Written in Fortran-4 for the IBM-360/75 computer. Multi-level cross section calculation in R-matrix formalism for l = 0 to 3 with Doppler broadening. Gives $\sigma_{n,T}$, $\sigma_{n,n}$, $\sigma_{n,\gamma}$ but not in UKNDL format.
	12. _____	Written in Fortran-4 for the IBM-360/75 computer. Similar to MLCSC and includes $\sigma_{n,f}$ for l = 0 only.
	13. SIGAV(*)	Written in Egtran-2(1) for the KDF-9 computer. Calculates averaged $\sigma_{n,T}$, $\sigma_{n,n}$, $\sigma_{n,\gamma}$ from resonance statistical parameters for l = 0 to 4; at present only for spin 0 target nuclides.
	14. CWF(*)	Written in Egtran-2(1) for the KDF-9 computer. Calculates coulomb penetration and shift factor for l = 0 to 5.
	15. OPW(*)	Written in S-2(2) for the IBM-7030 computer. Optical model; includes a fast search routine for parameter fitting.
	16. HFW(*)	Written in S-2(2) for the IBM-7030 computer. Hauser-Feshbach calculations with option for Moldauer correction.
	17. SCORE	Written in Fortran-4 for the IBM-360/75 computer. Uses IBM-2250 CRT console for computer-interactive-graphic display of NEUDADA and ENDF/B data files with output in UKNDL format.

- - - - - - - - - - - -

(1). Egtran-2 is a dialect of Fortran-2 developed for the KDF-9 computers.

(2). S-2 is a dialect of Fortran-2 developed for the old IBM-7030 computer. The programmes OPW and HFW have probably been converted to Fortran-4 for the IBM-360/75.

Table VI.

Computer Programmes For Format Conversion From One Evaluated Data Library to Another

Programme	Translation From	Translation To	Member State (Laboratory) of Origin
———	ENDF/B	KEDAK	Belgium (C.E.N./Mol). Programme just completed
UKTOA	UKNDL	ENDF/A	Japan (J.A.E.R.I.). Report JAERI-Memo-3162.
UKE	UKNDL	ENDF Formats	U.S.A. (O.R.N.L.). Report ORNL-TM-2880 (ENDF-134).
KTOE	KEDAK	ENDF/B	Italy (C.D.C.). Programme operational.
ETOS	ENDF/B	SPENG	Sweden (A.E.). Converts from ENDF/B to the Swedish SPENG library which contains effective group and point cross sections. This programme has just been completed.
UTOE	UKNDL	ENDF/B	Italy (C.D.C.). Programme operational.
UK-LRL	UKNDL	LLL	U.S.A. (L.L.L.)
LRL-UK	LLL	UKNDL	U.S.A. (L.L.L.)
ENDF-LRL	ENDF/B	LLL	U.S.A. (L.L.L.)
UKEL	LLL	ENDF/B	U.S.A. (L.L.L.). This programme is a modified and extended version of the UKE code.
———	KEDAK	UKNDL	France
———	ENDF/B	UKNDL	U.K. (A.W.R.E.). Development and testing of programme continuing. Programme is in Fortran-4 for the IBM-360/75 computers.
———	UKNDL	U.S.S.R. Format	U.S.S.R. Programme completed.
———	KEDAK	U.S.S.R. Format	U.S.S.R. Programme nearing completion.
———	ENDF/B	U.S.S.R. Format	U.S.S.R. Work just begun on this programme.
———	SPENG, KEDAK, ENDF/B	UKNDL	U.K. Various programmes have been written ad hoc, to perform piecemeal conversions from these libraries to the UKNDL format.

Table VII.

Institutes Involved in the Evaluation Effort.

Member States	Institutes
Australia	1. Australian Atomic Energy Commission's Research Establ. 2. University of Melbourne 3. University of Wollongong
Belgium	Centre d'Etudes Nucléaires, Mol
Bulgaria	Bulgarian Academy of Sciences, Institute of Physics and Nuclear Research Centre
Canada	Atomic Energy of Canada Ltd. (Chalk River)
France	1. Centre d'Etudes Nucléaires, Saclay 2. Centre d'Etudes Nucléaires, Cadarache 3. Centre d'Etudes Nucléaires, Limeil 4. Centre d'Etudes Nucléaires, F.A.R.
Fed. Rep. Germany	Gesellschaft für Kernforschung G.m.b.H., Karlsruhe
Hungary	1. Institute of Experimental Physics, Kossuth University 2. Central Research Institute for Physics, Budapest
India	Bhabha Atomic Research Centre
Israel	1. Soreq Nuclear Research Centre 2. Israel Institute of Technology, Technion
Italy	Centro di Calcolo, Bologna
Japan	1. Japan Atomic Energy Research Institute 2. Mitsubishi Atomic Power Industries Inc. 3. Nippon Atomic Industry Group Ltd. 4. Sumitomo Atomic Energy Ltd. 5. Kyushu University

Netherlands	Reactor Centrum Nederland
Romania	Institute of Atomic Physics
Sweden	1. AB Atomenergi 2. Research Institute of the Swedish National Defense
U.S.A.	1. Atomics International Inc. 2. Los Alamos Scientific Laboratory 3. Lawrence Livermore Laboratory 4. Oak Ridge National Laboratory 5. Brookhaven National Laboratory 6. Westinghouse Advanced Reactors Division Ltd. 7. Babcock and Wilcox Inc. 8. Idaho Nuclear Corporation 9. W.A.D.C.O. 10. Argonne National Laboratory 11. General Electric (San José) 12. Gulf General Atomic Co. 13. Batelle North-West Laboratories
U.K.	1. Atomic Energy Establishment, Winfrith 2. Atomic Weapons Research Establishment, Aldermaston 3. Atomic Energy Research Establishment, Harwell
U.S.S.R.	1. Institute of Physics and Power Engineering, Obninsk 2. Institute of Theoretical and Experimental Physics, Moscow 3. Institute of Nuclear Research of the Byelorussian SSR Academy of Sciences, Minsk 4. Institute of Nuclear Research of the Ukrainian SSR Academy of Sciences, Kiev.

Fig. 1.

The Neutron Nuclear Data Cycle.

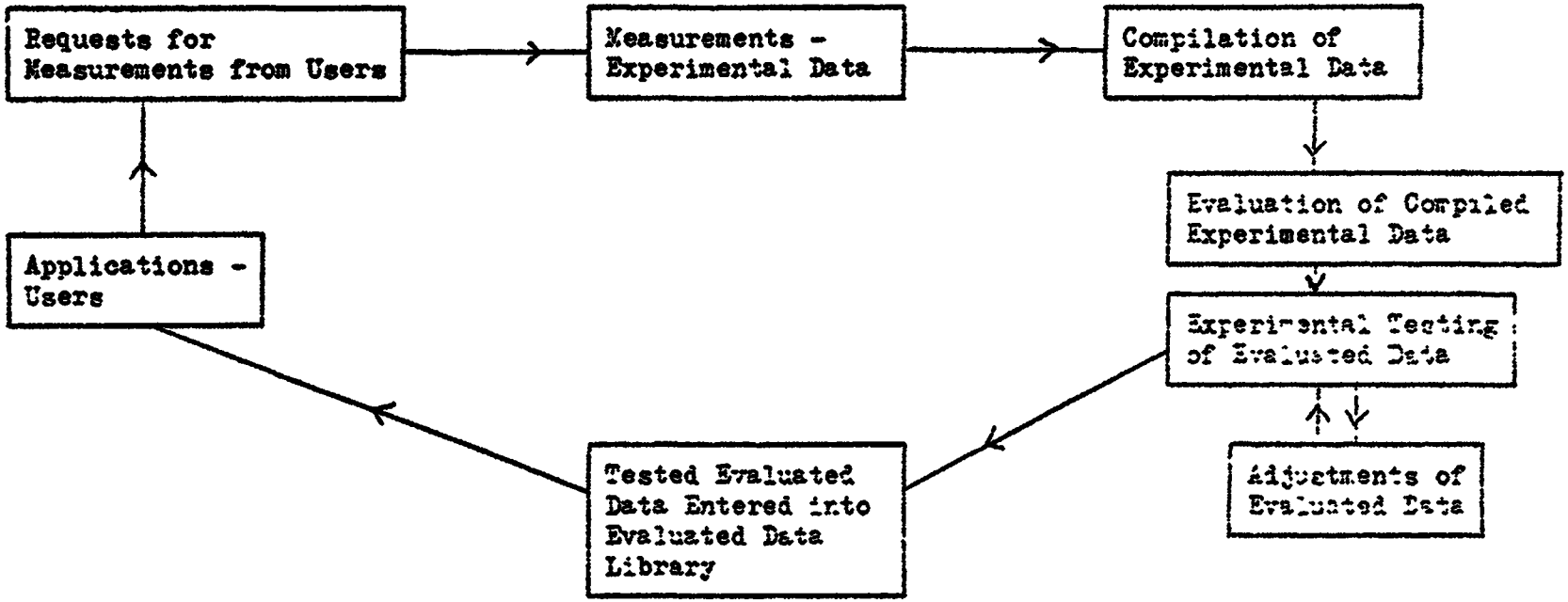
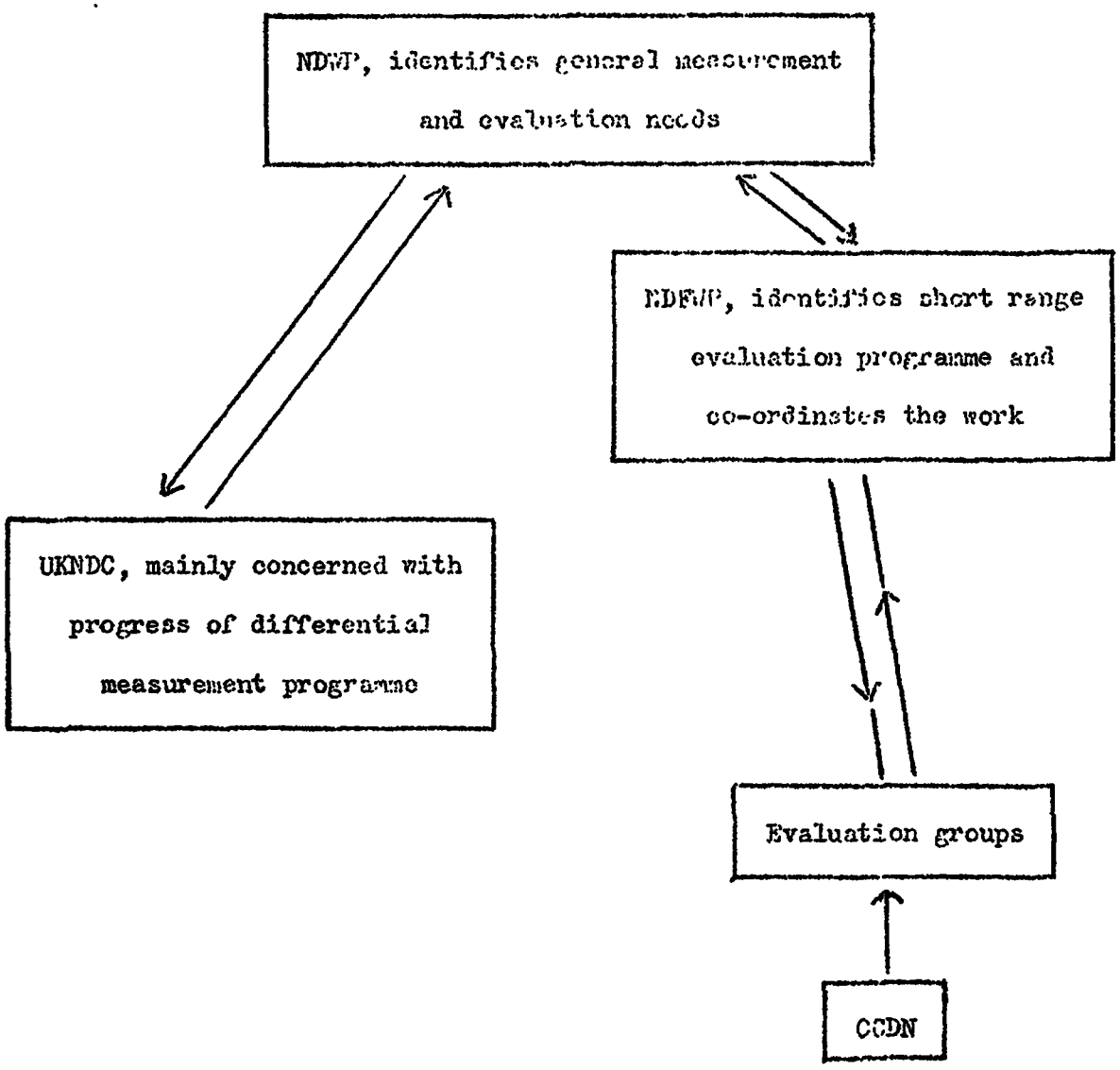


Fig. 11.

United Kingdom of Great Britain and Northern Ireland

Organisation and co-ordination of the national evaluation effort

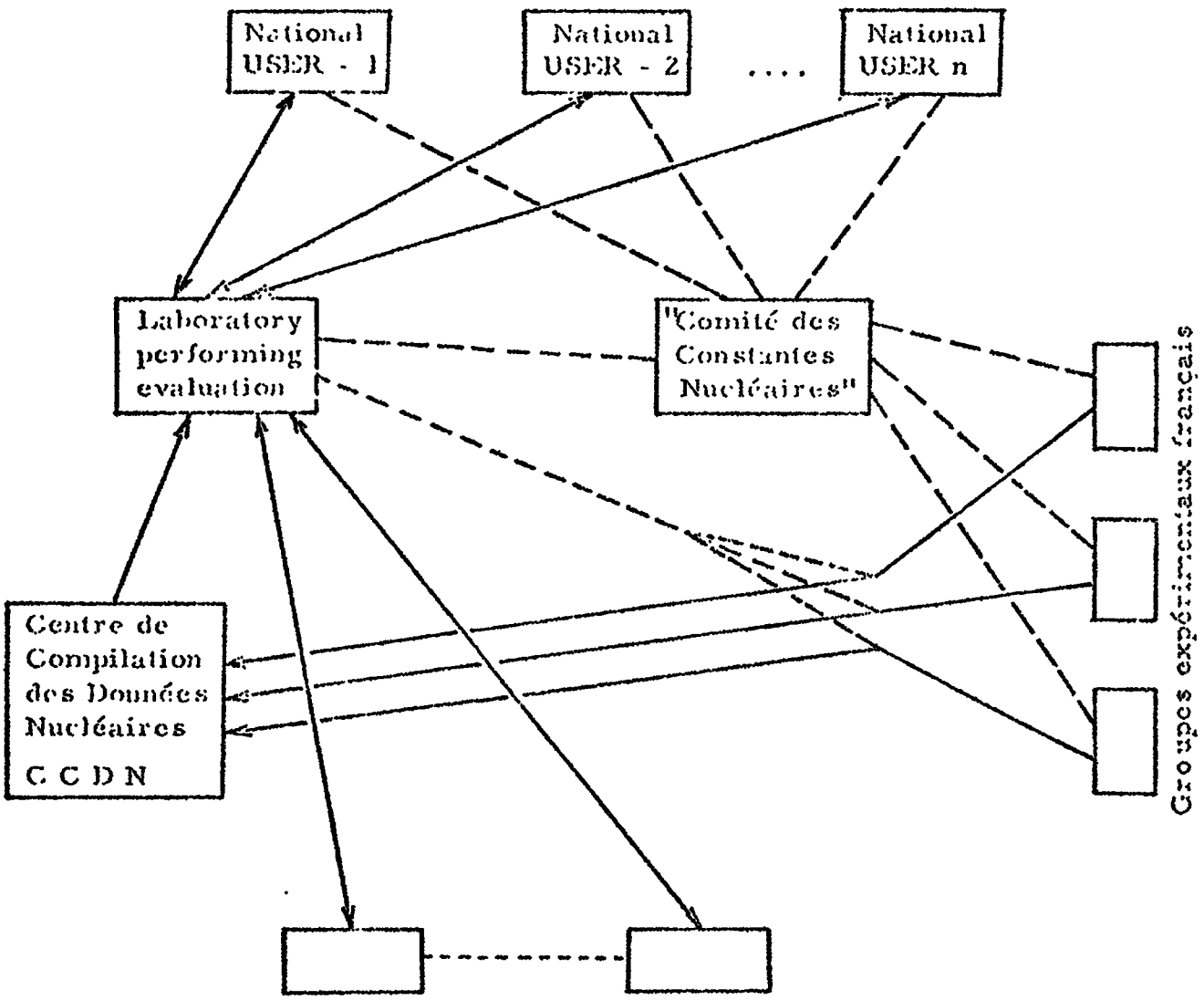


NDWP - Nuclear Data Working Party
NDFWP - Nuclear Data Files Working Party
CCDN - ENEA Neutron Data Compilation Centre, Saclay
UKNDC - United Kingdom Nuclear Data Committee

Fig. III

France

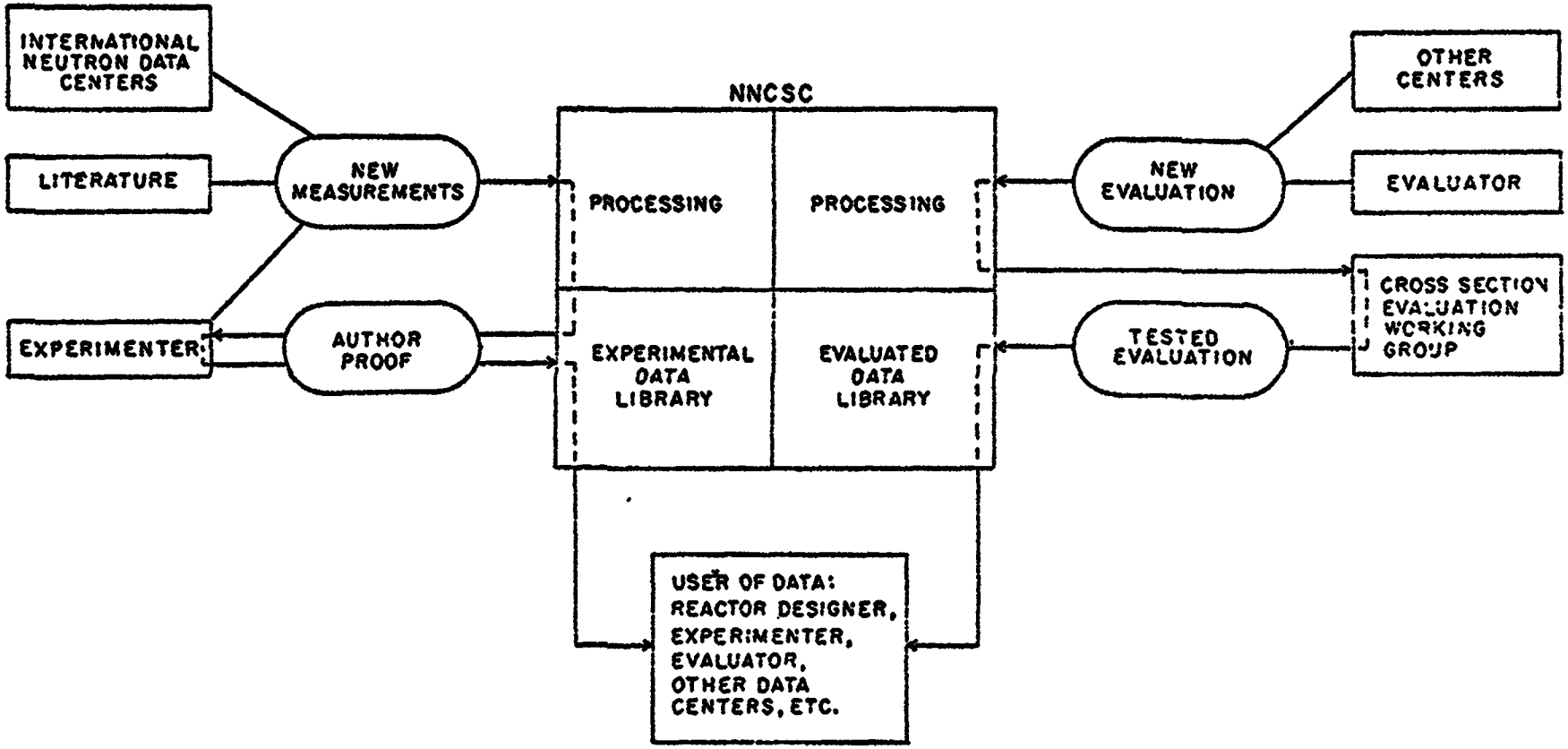
Organisation and Co-ordination of National Evaluation Effort.



Others evaluation groups in the would, mainly in Europ

Fig. IV.

U.S.A.

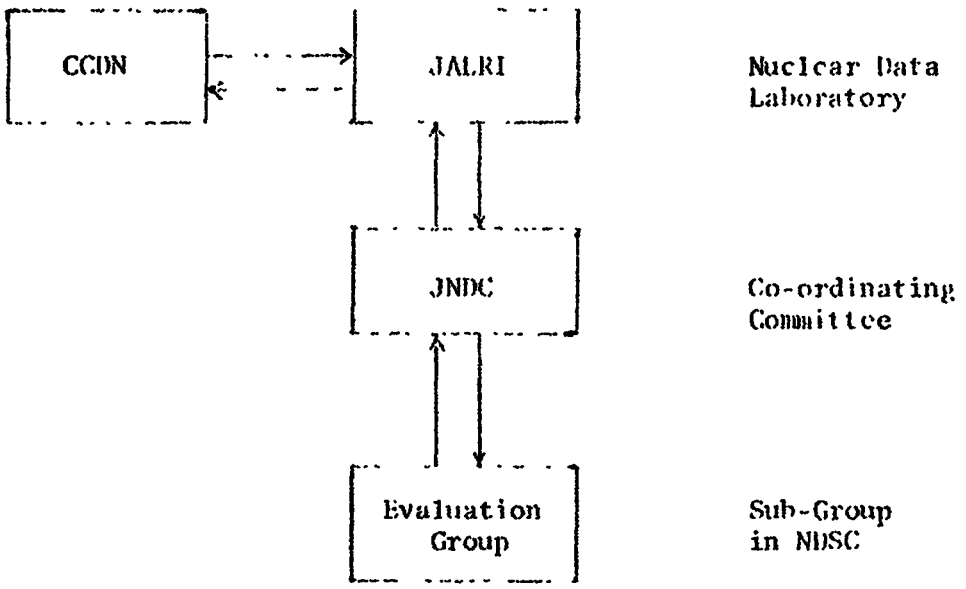


NNCSC - National Neutron Cross Section Center

Fig. V.

Japan

Organization and Co-ordination of National Evaluation Effort.



JNDC < NDSC
RCSC

JAERI (Japan Atomic Energy Research Institute)

JNDC (Japanese Nuclear Data Committee)

NDSC (Nuclear Data Sub-Committee)

RCSC (Reactor Constant Sub-Committee)

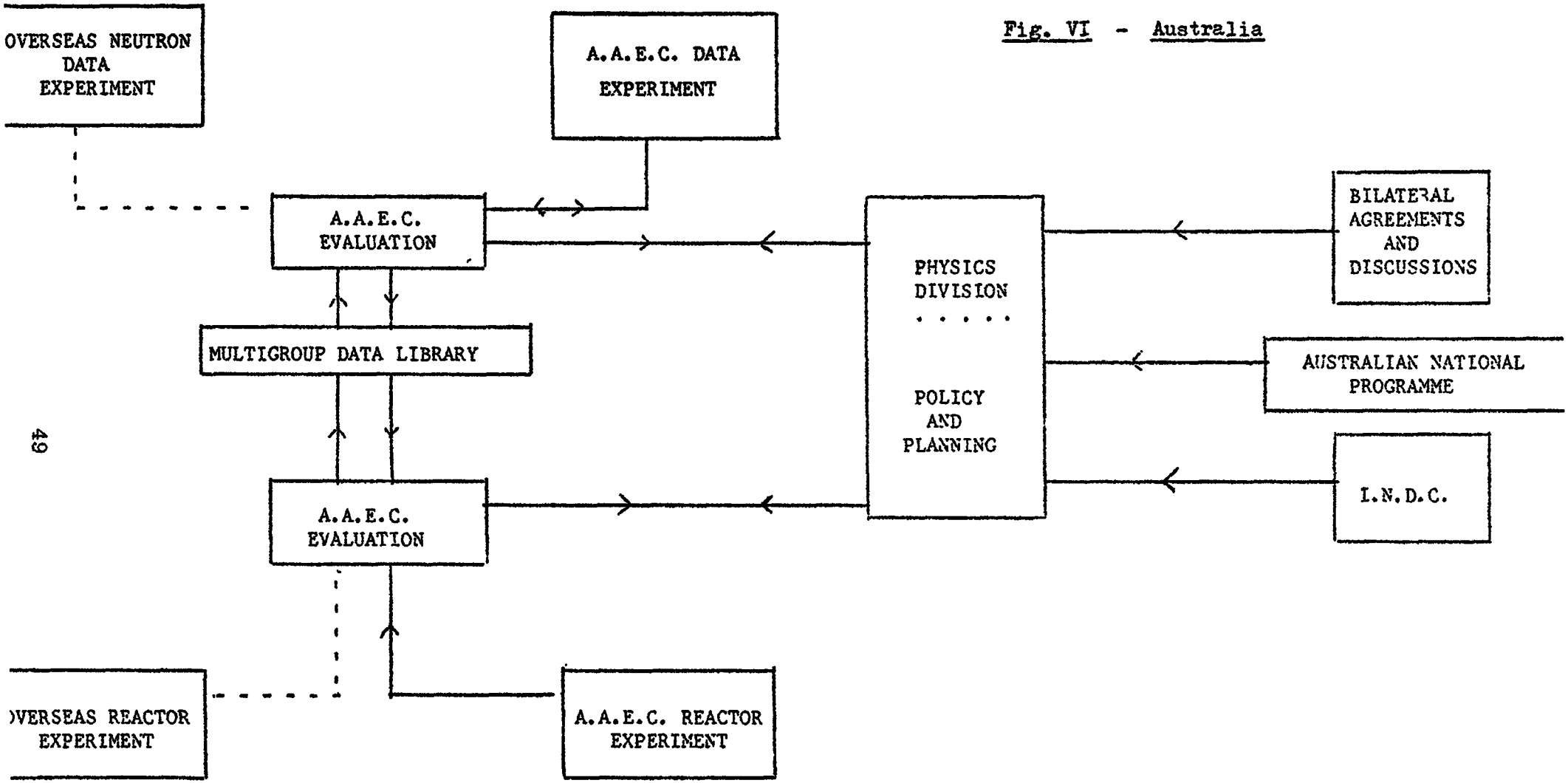
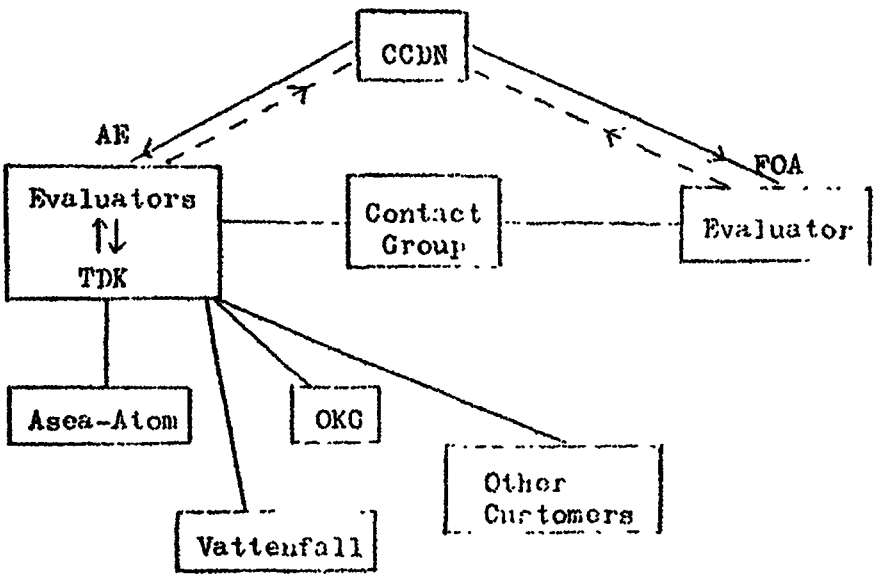


Fig. VI - Australia

A.A.E.C. - Australian Atomic Energy Commissio
I.N.D.C. - International Nuclear Data Committ

Fig. VII.

Sweden



AE - AB Atomenergi

FOA - Research Institute of the Swedish National Defense

TDK - Cross Section Data Committee

OKG - Oskarshamns Kraftgrupp AB

CCDN - ENEA Neutron Data Compilation Center, Saclay

ANNEX I

Circular Letter of 11 May 1971

Dear

In accordance with the recommendation of the International Nuclear Data Committee, the International Atomic Energy Agency will convene a panel of experts on the subject of Neutron Nuclear Data Evaluation at the Agency's Headquarters in Vienna from 30 August to 3 September 1971. The objectives of the panel are to review the methods, quality and present status of neutron nuclear data evaluation, as well as to examine the basic requirements and problems associated with establishing and exchanging evaluated neutron data libraries. The panel will be asked to report to the Director General of the Agency on the current status of the topics discussed and to recommend guidelines for the Agency's future programme in this regard. The Provisional Agenda for the panel is attached.

For the first item of the Provisional Agenda, the Nuclear Data Section will prepare a review of the neutron data evaluation activities, the important evaluation needs and the assessment of these needs in Member States. The success of this review clearly depends upon the relevant information being made available to the Agency. In this context we would greatly appreciate if you could complete the questionnaires in Annexes I and II and supply any other pertinent information on the evaluation activities and/or evaluation needs in your country. If you are not in a position to supply us with the relevant information, we would greatly appreciate if you forward this letter to the appropriate person(s) for action.

So as to allow sufficient time for the completion of this review prior to the panel, we would urge you to send us your reply as soon as possible so as to reach us not later than 9 July 1971. If you need any further clarification regarding the contents of Annexes I and II, please feel free to contact us immediately.

Thanking you for your cooperation,

Yours sincerely,

Enclosures

J.J. Schmidt, Head
Nuclear Data Section
Division of Research
and Laboratories

Annex I

I. Review of the Important Neutron Data Evaluation Needs and the Assessment of these Needs in Member States

The information required under this item is related to the following four questions:

1. How does your country go about identifying its neutron data evaluation requirements ?

2. Who are the users of evaluated neutron data in your country ?

3. How far do the existing evaluated neutron data libraries meet the needs of the users in your country ?

4. For those Member States that do not have a neutron data evaluation programme, what are the needs for such data in your country ?

Annex II

II. Review of the Neutron Nuclear Data Evaluation Activities in Member States

Under this item information related to four basic questions is required:

1. The neutron data evaluation work in progress at present and that which will be started before the end of 1971 ? - (Specimen reply given in Table II.1).

2. The computer programmes and codes available ? - (Further specifications given in Table II.2).

3. The Laboratories/Institutes involved in the evaluation effort (Tables II.1 and II.3); the organization and co-ordination of the evaluation work between these Laboratories/Institutes (Table II.4) and the total manpower available for the evaluation effort (Table II.3) ?

4. Does your country collaborate, bilaterally or multilaterally, with other States in co-ordinating, organizing and performing evaluations ? If so, please indicate in what form (e.g., contracts, committees, newsletters) and on what subjects does this collaboration manifest itself.

Table II.1

Work in Progress (I) and Work Planned (II) during the next 6 months.

Nuclide	Cross Section Type	Energy Range	Evaluators' Names (Laboratory)
Pu-239 (I)	α, $\bar{\nu}$, σ_f	Thermal - 15 MeV	..... (...)
U-238 (II)	All reaction types	1 KeV - 20 MeV	..... (...)
Au-197 (II)	$\sigma_{n,\gamma}$	1 KeV - 10 MeV	..... (...)
Na (I)	All reaction types	1 KeV - 15 MeV	..... (...)
Fission Products	$\sigma_{n,\gamma}$	1 KeV - 10 MeV	..... (...)

Table II.2

A. What computer facilities are available for performing evaluations and for handling evaluated data libraries ?

B. What evaluated neutron data libraries are used in your country and what are their formats ?

C. What are the contents of these libraries ?

D. What computer programmes and calculational codes are available for:

1. Evaluated data handling (e.g., checking, editing, updating, etc.) ?

2. The analysis and calculation of cross-sections ?

3. Format conversion from one evaluated data library to another ?

Table II.3

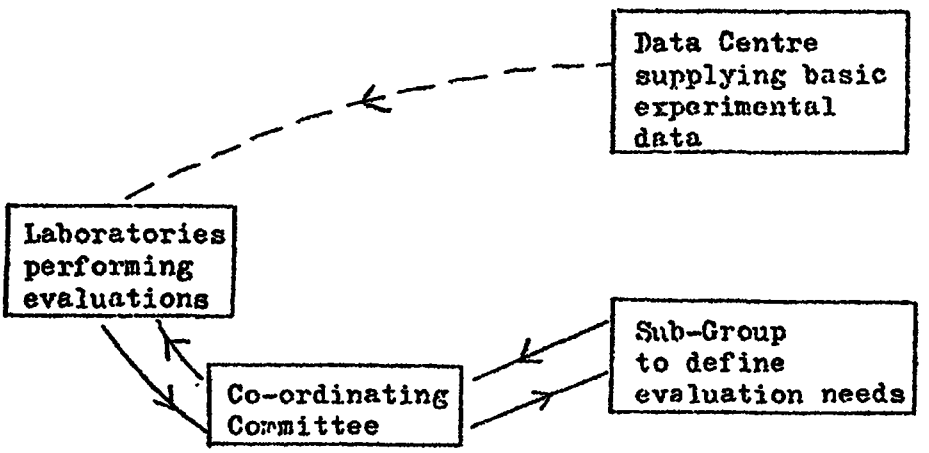
Laboratories/Institutes Involved in the National Evaluation Effort and the Manpower Available to Support this Effort

Laboratory/Institute	Total Manpower Available for Evaluation (man-months of post-graduate staff)	
	at present	in 1972

Table II.4

Organization and Co-ordination of National Evaluation Effort.

The chart below gives a schematic outline of a possible organization of a national neutron data evaluation programme. We would appreciate it if you could draw up the chart valid for your country.



Annex II.

Extract Submitted by Sweden from the Report: -

" A Computer Programme for Calculation of Neutron Spectrum and (Fast Reactor) Group Cross Sections in a Finite Homogeneous Medium ",
by K. Nyman, AE-RFN-279 (1967).

General rules for punching data are given in the section "General Rules for Input Data".

If generation or updating of the library data tape is included in the run the corresponding data must be stacked first in the data deck. The principles for arranging data for a type 1 or a type 2 phase differ somewhat from the rules for the other phases. Therefore the description of the input data etc for these phases is contained in a separate chapter, and the description for the other types of phases forms the next chapter.

III. 1. General Rules for Input Data

The input to Speng is format-free. That means that the position of a quantity (a number or a word etc) on the card is unimportant, as is the number of cards used. The only requirements are 1) that the quantities should be punched in the correct order, and 2) that they shall be separated from each other by at least one blank. A quantity cannot extend over two cards (the code puts a blank in an imaginary column 81). There are a few exceptions to this. The current input card image is lost, when a new program link is entered in the computer storage. Therefore the punching must start on a new card after each data group, that causes such a change of program link. The occations are few and are expressly stated in the sections, that deal with the arrangement of the data.

A comma affects that everything punched to the right of it is ignored. This fact can be used to insert notations on the data cards. E g the notation for the element could be punched after a comma on each card containing microscopic data for that element. The insertion of a comma after the last significant information on a card also releases the code from converting the rest of the card from BCD to binary and thus saves computer time.

Five types of quantities appear in the data:

1. Integers — An integer consists of decimal digits without a decimal point, it may be signed or unsigned.

2. Real numbers — A real (floating point) number consists of decimal digits. It may include a decimal point at the beginning, at the end or between two digits. A real number can be followed by a decimal exponent that is written as the letter E followed by the exponent. There must be no blank field between the real number and the letter E. Blanks may, however, separate the letter E and the exponent. A number that is not explicitly classified as an integer in this description is a real number.

3. Words — A word is a combination of letters. Only the first six characters of a word are significant to the code, but the remaining characters must all be letters too. The words are used as directives or headings in the data. In some cases a directive is formed by writing two or more words as one word. (E g TRANSPORTGROUPS must not be written as TRANSPORT GROUPS but can be shortened to TRANSP).

4. Special words or notations for elements or isotopes and for materials — Such a notation is a combination of letters and figures with a letter as the first character. E g AL13, FE26B. Only the first six characters are significant.

5. x — The asterisk.

The exact images of all input cards are printed successively as they are read. Each occupies one line, which ends with the words "DATA CARD". Thus all input data are recorded.

III. 2. Restrictions and Error Messages

Some restrictions on the length of data arrays are indicated in the following sections. If such a restriction is violated the programme prints an error message and the run is automatically interrupted.

The programme also tests for and prints error messages at a large number of other data errors. Normally then the execution is stopped. But if an error is detected when reading data for an element or an isotope the input of data continues with the data for the next element instead.

A syntactical error in the data is almost always detected by the programme.

The amount of element data (see below) that can be stored is limited by the capacity of one magnetic tape. This capacity depends upon the effective length of the tape and of the character density used. The magnitude is of the order of one or two million numbers.

The neutron spectra are also all stored on one magnetic tape. Only a very samll portion of a magnetic tape will ever be made use of for that purpose. The monitor system provides a test and prints an error message if the "end of tape condition" is encountered.

III. 3. Preparation of Data for the Generation or the Updating of the Element Data tape etc.

The library data tape holds the atomic weights, microscopic crossections and all other data specific to elements, that are needed for the calculations. A joint name for these data in this report is "element data".

The tape is generated and updated by the programme and during a calculation the crossection values etc are always taken from the data tape.

The bulk of the data for a generate or an update phase are a number of data decks, each holding the element data for one element. Punching specifications for such a deck are given in the first sub-chapter.

A few data groups or directives are also needed to control the execution of a generate or an update phase. They are described in the next sub chapter. Finally the arrangement of the data for a generate or an update phase is specified in one sub-chapter.

III. 3. A. Punching specifications for "element data"

In this sub-chapter all data groups that belong to a data deck for an element are described in the same order as they shall be stacked within the deck.

ELEMENT ide a bnn bn2n ann
an2n c1 c2 . . . . . ck

ide is the notation for the element. It is a combination of letters and figures with a letter first - a type 5 quantity. E g FE26 or U28B2. There must be no blank between the first and the last character of the notation.

a is the atomic weight.

bnn and bn2n are the thresholds for the nn′- and the n2n-reaction respectively. ann and an2n are parameters in a statistical model for nn′- and n2n-scattering.

c1, c2, ... ck are classification numbers (integers) for these and only these crossections, which are tabulated under the heading "CROSSECTIONS" below. Their interpretations are: 1 (one) total crossection, 2 (two) elastic-, 4 (four) total nn′-, 16 (sixteen) n2n-, 18 (eighteen) fission- and 101 (one hundred and one) capture-crossection.

The classification numbers are punched in the same order as the corresponding crossection values are given later on.

TEMPERATURES t_1 t_2 . . . . . t_p

This data group is necessary only if temperature dependent crossections occur under "CROSSECTIONS" (see below).
t_1, t_2, ... t_p are the temperature values in degrees Kelvin in ascending order.

Restriction: The number of temperatures must not exceed 6.

BACKGROUNDVALUES b_1 b_2 . . . . b_q

The heading shall be punched as one word. This data group shall be included if and only if (temperature- and background-dependent) effective crossections occur under "CROSSECTIONS" (see below). b_1, b_2, ... b_q are the background values in barns, in ascending order.

Restriction 1: The number of background values must not exceed 12.

Restriction 2: The maximum number of shieldable elements in one mixture is 6.

THRESHOLDS ϵ_1 ϵ_2 . . . . . ϵ_t

This data group is necessary if partial nn′-crossections for separate levels will be given under "CROSSECTIONS".
ϵ_1, ϵ_2 . . . . . ϵ_t are the levels in MeV in ascending order.

Restriction: The number of levels must not exceed 15.

FISSILE

See below.

FERTILE

The element shall be classified as fissile or fertile, if the fission crossection is non-zero.

NUMBEROFNEUTRONSPERFISSION e_1 $\nu(e_1)$ e_2 $\nu(e_2)$ . . . . . e_n $\nu(e_n)$

The heading is punched as one word. This data group shall be included, if and only if the fission crossection is non-zero. $\nu(e)$ is the number of neutrons per fission at energy e.

Restriction: The number of energy values must not exceed 25.

DELAYEDNEUTRONYIELD dny

The heading is punched as one word. This data group shall be included, if and only if the fission crossection is non-zero. One value dny represents the delayed neutron yield for all energies.

CROSSECTIONS

Crossection values for one energy point or one fine-group at a time in order of decreasing energy. The data for each energy point or energy group being arranged as described below.

If a kind of crossection (say the n2n-crossection) is included in the table, the corresponding classification number (16 for n2n) must occur above under "ELEMENT" and vice versa.

The table must cover the energy regions, that will be concerned in the calculations. If a calculation of a neutron spectrum

or of group crossections will be performed for $E_{min} \leq E \leq E_{max}$, it is required, that the crossection tables for all elements, that are concerned, extend up to $1.001 \times E_{max}$ and down to $0.999 \times E_{min}$.

For most energies temperature independent crossection values are accurate. But the crossections at an energy or for a fine group in the resonance region may also be represented by temperature dependent functions or by temperature - and background dependent effective values.

Energy values are given in MeV, crossection values in barns and temperature values in degrees Kelvin.

A minus sign before an energy value indicates that the crossection values that follow are "group crossections". The minus sign and the energy value must not be separated by intervening blanks. The group extends from the energy value, that precedes the crossection values, up to the next higher energy value, that precedes the preceding set of crossection values in the table. The absence of a minus sign before an energy value indicates, that the crossection values that follow are "point crossections". The table must start with a positive "energy" value.

The number of energy-points or fine-groups is limited only by the fact that one magnetic tape must take all the data for all elements.

Two tests are done on the consistency of the crossections.

1. At each point of tabulation the code checks whether
$$\left|[\sigma(\text{TOTAL}) - \sigma(\text{ELASTIC}) - \sigma(N,N') - \sigma(N,2N) - \sigma(\text{FISSION}) - \sigma(\text{CAPTURE})]/\sigma(\text{TOTAL})\right| < 0.0001$$

2. If σ_e-values are given at the point of tabulation or at a higher energy, the code checks whether
$$\left|\left\{\sigma(N,N') - \sum_{i=1}^{t} \sigma_{ei}\right\}/\sigma(N,N')\right| < 0.0001$$

If the tolerance is exceeded, an error message is printed and the data are not stored.

1. Temperature independent crossections.

e_n	$\sigma^{c1}(e_n)$	$\sigma^{c2}(e_n)$ . . . . . $\sigma^{ck}(e_n)$

The crossection values are given in the same order as the corresponding classification numbers c1, c2, ... , ck are given above under "ELEMENT".

If e_n is a positive number the σ:s are interpreted as "point crossections" at energy e_n. If e_n is a negative number the σ:s are interpreted as "group crossections". Then $/e_n/$ is the lower group boundary, and the upper boundary equals the next higher energy value $/e_{n-1}/$ in the table. This may be either the lower boundary of another group or - if e_{n-1} is positive - the energy corresponding to "point crossections".

If partial nn′ - crossections for separate levels are known at this energy, they may be specified - preceded by an asterisk - after the other crossections. Thus

e_n	$\sigma^{c1}(e_n)$ . . . . . $\sigma^{ck}(e_n)$	* $\sigma^{\epsilon 1}(e_n)$
$\sigma^{\epsilon 2}(e_n)$ . .	. . $\sigma^{\epsilon t}(e_n)$	

The crossections are punched in order of increasing energy of the levels ϵ and one value must correspond to each level, that is specified under "THRESHOLDS".

If $\sigma_{nn'}(e_n)$ is non-zero, and if partial nn′-crossections are given for a higher energy than e_n (for this element), they must also be specified for e_n.

2. Temperature dependent crossections.

T			
e_n	t_1	$\sigma^{c1}(e_n,t_1)$	$\sigma^{ck}(e_n,t_1)$
e_n	t_2	$\sigma^{c1}(e_n,t_2)$	$\sigma^{ck}(e_n,t_2)$
. . . . .			
. . . . .			
e_n	t_p	$\sigma^{c1}(e_n,t_p)$	$\sigma^{ck}(e_n,t_p)$

The letter "T" indicates that the crossections at the energy e_n or - if $e_n \neq 0$ - for the fine-group $/e_n/ \geq E \geq /e_{n-1}/$ are tabulated as temperature dependent functions.

$t_1, t_2, \ldots, t_p$ are the temperature values. They shall equal in number, order and - within a small tolerance - in magnitude the values, that are given under "TEMPERATURES". The same value e_n shall be repeated before each temperature value.

Only the total-, the elastic-, the capture- and the fission-crossection may vary with the temperature. If the nn'- and/or the n2n-crossection is (are) punched the same value(s) must be repeated for each temperature value.

If partly partial nn'-crossections are specified for a higher energy than $/e_n/$ for this element and partly $\sigma_{nn'}(e_n) \neq 0$, these data shall be followed by

x	$\sigma^{\epsilon 1}(e_n)$	$\sigma^{\epsilon t}(e_n)$

3. Temperature- and background-dependent effective crossections.

TB			
e_n	t_1	b_1	$\sigma^{c1}(e_n,t_1,b_1) \ldots \sigma^{ck}(e_n,t_1,b_1)$
e_n	t_1	b_2	$\sigma^{c1}(e_n,t_1,b_2) \ldots \sigma^{ck}(e_n,t_1,b_2)$
. . .	. . .	. . .	. . . . .
e_n	t_1	b_q	$\sigma^{c1}(e_n,t_1,b_q) \ldots \sigma^{ck}(e_n,t_1,b_q)$
e_n	t_2	b_1	$\sigma^{c1}(e_n,t_2,b_1) \ldots \sigma^{ck}(e_n,t_2,b_1)$
. . .	. . .	. . .	. . . . .
. . .	. . .	. . .	. . . . .
e_n	t_p	b_q	$\sigma^{c1}(e_n,t_p,b_q) \ldots \sigma^{ck}(e_n,t_p,b_q)$

If partly partial nn'-crossections are specified for a higher energy than $/e_n/$ for this element and partly $\sigma_{nn'}(e_n) \neq 0$, these data shall be followed by

x	$\sigma^{\epsilon 1}(e_n) \ldots \sigma^{\epsilon t}(e_n)$	

The "TB" indicates that the crossections for the fine-group $/e_n/ \leq E \leq /e_{n-1}/$ or - if $e_n > 0$ - at the energy e_n are tabulated as temperature and background dependent functions. No blank may separate the letters. Background dependent crossection values may occur in the tables only in the energy region 1 eV - 100 keV.

$t_1, t_2, \ldots, t_p$ are the temperature values and $b_1, b_2, \ldots, b_q$ are the background values. They shall equal in number, order and - within a small tolerance - in magnitude the values that are given under "TEMPERATURES" and "BACKGROUNDVALUES" respectively. The same value e_n shall be repeated before each pair of values t and b. The second, third etc e_n-value and the t- and b-values are only used to check the internal order of the cards.

The crossection values shall be given in the same order as the corresponding classification numbers c1, c2, ..., ck are given under "ELEMENT". Only the total-, the elastic-, the capture- and the fission-crossection may vary with the temperature and the background value. The same nn' -value and the same n2n-value must be repeated for each pair of values t and b, if these crossections are included in the crossection table.

It is checked during input of the data, that the crossection values do not decrease with increasing background value. During a calculation it is checked, that the effective crossections do not decrease with rising temperature.

LEGENDRECOEFFICIENTS k e_1 $f_1(e_1)$ $f_2(e_1)$ . . . . . $f_k(e_1)$ e_2 $f_1(e_2)$ $f_2(e_2)$ . . . . . e_n $f_1(e_n)$ $f_2(e_n)$ . . . . . $f_k(e_n)$

The heading is punched as one word. k is the number of coefficients (an integer). The energies e_i should be given in MeV in monotonously decreasing order. The relative coefficients f in the legendre expansion of the angular distribution of elastically scattered neutrons shall be given in the centre of mass system. The tabulation of the legendre coefficients must extend up to 1,001 times the highest energy, that will be concerned in the calculations. It is interrupted when all coefficients equal zero.

Restriction 1. The number of coefficients must not exceed 10.

Restriction 2. The number of (non-zero) values in the whole table is restricted by the inequelity

$$2n + \sum_{i=1}^{n} k_i \leq 990$$

Here $k_i \leq k$ is defined by

$$f_\ell(e_i) \neq 0 \text{ for } \ell = k_i$$

$$f_\ell(e_i) = 0 \text{ for } \ell > k_i$$

Note. If a crossection or a legendre-coefficient etc is zero, it is sufficient to punch only the figure "0".

END

The directive word END ends the data for one element.

Arrangement of the Data for one Element or Isotope

The internal order of the directives and the data groups within a data deck for one element shall be

"ELEMENT etc . . . . . "	
"TEMPERATURES etc . . . . . "	(see below)
"BACKGROUNDVALUES etc . . . . "	(see below)
"THRESHOLDS etc . . . . . "	(see below)
"FISSILE" or "FERTILE"	(see below)
"NUMBEROFNEUTRONSPERFISSION etc . . . "	(see below)
"DELAYEDNEUTRONYIELD etc . . . "	(see below)
"CROSSECTIONS etc . . . . . "	
"LEGENDRECOEFFICIENTS etc . .. "	
"END"	

Data group "TEMPERATURES etc . . . " shall be included (only) if some crossections are temperature dependent.

Data group 'BACKGROUNDVALUES etc . . . " shall be included (only) if background dependent effective crossection values occur under "CROSSECTIONS".

Data group "THRESHOLDS etc . . . " must be specified if nn'-crossections for separate levels are tabulated.

Data groups "FISSILE" or "FERTILE" and "NUMBEROFNEUTRONSPERFISSION" etc . . . " and "DELAYEDNEUTRONYIELD etc . . . " shall be included, if and only if the element has a non-zero fission crossection.

Annex III.

Preliminary List of Requests for Neutron Data Evaluations

Submitted by Sweden.

AB Atomenergi

Isotope or Element	Priority	Type of evaluation requested and comment
O	I	All cross sections taking in consideration weaknesses found in ENDF/B data for oxygen
F	III	
Si	II	Can probably wait evaluation in progress at BNL
Si(n, α)	III	Best value of (n, α) curve considering recent measurements (Grimes for instance)
Ti46(n,p)	II	Best value of (n,p) curve considering recent measurements (Lukac NSE 43, 233, Ghoray BAPS 15, 1329)
Mn(RI abs) (thermal)	II	Best thermal abs. cross section and R I abs. value
Fe	I	Assemble a "best" data set from existing evaluations, including a set of resonance parameters to calculate cross sections in resonance region
Ni	I	Specially (n,α) evaluation including set of resonance parameters to calculate cross sections in resonance region (Moxon eval. extends up to 200 keV)
Cu	III	reevaluation in resonance region specially considering recent measurements at Geel and KFK
Ag(RI abs) (thermal	II	Best thermal absorption and RI value for use with activation detectors
Pu239	II	Set of p-wave resonance parameters
Pu240	II	Set of p-wave resonance parameters

FOA

N	II	}	γ-production
O	II	}	thermal to 15 MeV

Neutron data evaluation studies in the United Kingdom in the second half of 1971

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Abstract

A brief outline of the organization of the neutron data evaluation and measurement programme in the United Kingdom is presented. The paper then summarizes in a qualitative manner the degree to which each of the complete files of the U.K. Nuclear Data Library (UKNDL) meets the current needs of users in the U.K. A more detailed review of the present and planned U.K. evaluation activities is subsequently presented along with a summary of the principal computer programmes used for the manipulation of evaluated data, as well as for the analysis and calculation of neutron cross sections.

1. Review of the important neutron data evaluation needs and the assessment of these needs in the United Kingdom

(i) At the present time there are three bodies in the United Kingdom dealing with differential nuclear data. The Nuclear Data Working Party (NDWP), chaired by C. G. Campbell of the Reactor Group, AEE Winfrith, meets on an ad hoc basis to collate and screen the UK nuclear data "Request List", to keep it up-to-date and to make recommendations on the priorities of new differential measurement work. It acts in an advisory capacity to the Physics of Reactors Research Committee which is responsible for formal approval of the Request List and for the measurement/evaluation programme. The membership of the NDWP is drawn from the UKAEA staff exclusively.

The Nuclear Data Files Working Party (NDFWP), also chaired by C. G. Campbell, has the main task of co-ordinating the UK evaluation work, especially as it applies to the production of computer files of nuclear data.

The UK Nuclear Data Committee (UKNDC) under the chairmanship of B. Rose, AERE Harwell, has the main task of co-ordinating the programme of differential data measurements. Most of the members of this committee are drawn from the UKAEA; the National Physical Laboratory is represented and other bodies, such as university departments, may be represented when appropriate. The UKNDC organises a Nuclear Data Forum, a one day symposium, once a year and taking place in turn at each of the various centres of measurement or user activity.

As an outcome of the development and growing use of the UK Nuclear Data Library (UKNDL) it has become increasingly recognised that users' requirements for new neutron data are most often requirements for new or revised evaluations in the UKNDL standard format. New experimental data may be needed also, but provision of these goes only half way towards meeting the users' requirements. Recently therefore there has been some shift in emphasis towards new evaluation work even at the expense of new measurements. It is expected that this will bring about an improved awareness of the main shortcomings in the data available and that it will benefit the experimental programme in the longer term. At the same time our nuclear data "Request List" has been split into two sections relating to new measurements and to new evaluation requirements, as a reflection of concern for improvement of evaluated data files.

The methods used to determine the accuracy requirements for cross-section data for thermal and fast neutron reactor calculations were described by G. H. Kinchin and R. D. Smith at the IAEA Paris conference on nuclear data for reactors in 1966. Some of the most important cross-sections cannot yet be measured to sufficient accuracy by differential methods, and it has proved necessary to institute a programme for data adjustment, which takes account of both differential and integral data to improve the accuracy of fast reactor performance predictions. This development was described by C. G. Campbell and J. L. Rowlands at the IAEA Helsinki Conference in 1970, and has much alleviated the demands for differential cross-section data of very high precision.

(ii) The main users of evaluated neutron data in the United Kingdom are the thermal and fast neutron fission reactor physicists and the Authority Health and Safety Branch. Some use of the data is being made for shielding calculations, and for radiation damage calculations. Recently too the fusion reactor physicists have begun to use the UK Nuclear Data Library, and to contribute to it.

(iii) Taking account of work in progress, data files are available in the UKNDL for almost all materials currently of interest for the UK reactor programme; for the most important materials the evaluations are up-to-date to within about 1 year - the accuracy of this latter group of data files is limited in the main by the uncertainties in the experimental data, at least insofar as the principal reactions are concerned. Multigroup cross-section sets in up to 2000 groups have been and are being produced from these files and are generally adjusted to give improved agreement with integral experiments.

Table 1.1 gives a somewhat more detailed view of the measure in which the UKNDL meets our users' current needs. Data files for some structural materials still need improvement, Cr and Mo for example. Many files of fission-product capture cross-sections are available, but they have not been extensively tested· many are known to be in need of improvement, and there is a need for average data on other reactions in bulk fission-products, elastic and inelastic scattering for example, and perhaps also for (n.p) and (n,α) reactions. Improved evaluations would be desirable for Am and Cm isotopes though it is probable that inadequacies in the experimental data are the main limitation. For many other

materials of lesser importance the data files stand much in need of careful revision and up-dating, and particular attention is called to the need for more careful assessments of the contributions by missed p- and d-wave resonances to neutron capture by elements in the low mass range, A ≈ 20 to 100.

2. Review of neutron nuclear data evaluation activities in the United Kingdom

(i) A considerable programme of evaluation work initiated towards the end of 1970 is nearing completion, but there remains much consequential "tidying-up" to be done - documentation, tape manipulations and checking, and so on. There are plans for converting a number of ENDF/B files to the UKNDL format: a computer programme has been developed for this work and is operational, but it is by no means fully tested yet, so that at present each conversion is still a laborious task involving much tape manipulation, checking and correction. With so much residual work to be accomplished, the programme of further data assessment work for the remainder of 1971 has not yet been formally identified, though work is in progress on Li^6, Cr, Mo, and Pu^{240}. Table 2.1 sets out our aspirations, however.

On the new evaluations or recent revisions mentioned in Table 1.1 the following comments may be of interest:-

The new file for D in D_2O follows, in the intermediate energy range, the conclusions presented by Story (AEEW) at the IAEA Helsinki conference on nuclear data for reactors 1, 721 (June 1970) - see Fig. 3 of that paper.

The new file for C follows a complete re-evaluation over the whole energy range 0.0001 eV to 15 MeV, by Douglas, Porter & Wyld (AWRE): documentation is in progress.

Work on Fe represents a complete re-evaluation of the resonance range, mainly by Pope & Story (AEEW). Parallel work on Ni has been carried out by Moxon (AERE). He concludes that the estimated uncertainty of the total cross-section is small in the range up to about 200 keV, and in the peaks of s-wave resonances the uncertainty is mainly that of the potential cross-section which is ± 0.5 barns at 1 eV and ± 2.0 barns at about 100 keV. The uncertainty in the capture cross-section varies from ± 5% in the 1/v region to between ± 10% and ± 30% in the vicinity of p- and d-wave resonances and about ± 50% in the s-wave resonances. Above 40 keV the average capture is given to about ± 30%.

The capture cross-sections of Kr^{83} and Pm^{147} were obtained from evaluations in the resonance range by Hammond & Story (AEEW), and at higher energies by Benzi et al. (CNEN, Bologna).

For U235, U238 and Pu239 nu-bar has been re-evaluated over the whole energy range by Mather & Bampton (AWRE); see AWRE O-44/71 and O-86/70 for U238 and Pu239 respectively. Above about 25 keV the fission cross-sections and the U238 capture cross-section have been revised using the "simultaneous fit" by Patrick & Sowerby (AERE)

and Mather (AWRE), of which a preliminary account was reported by Patrick & Sowerby at the IAEA Helsinki conference 2, 703 (1970). The GENEX tapes for these materials have also been brought into agreement with the "simultaneous fit" in the energy range below ·25 keV. The inelastic cross-section data for U^{238} and Pu239 and the (n,2n) and (n,3n) cross-sections of U^{238} have been re-evaluated by Douglas & Wylde (AWRE). Documentation of this work has been started.

(ii) The computer facilities and the principal programmes used for neutron cross-section data evaluation, and for handling evaluated data libraries are listed in Table 2.2.

In addition there is a suite of programmes associated with the GENEX data library; for details see Brissenden & Durston AEEW-R 622 (1968). The principal programmes are RESP and GENEX. RESP generates a sequence of resonance parameters by Monte Carlo selection from appropriate distributions. GENEX generates Doppler broadened cross-sections for capture, fission and scattering in a standard energy mesh, using the resonance parameters supplied by RESP. These programmes have been converted to Fortran-4 for the ICL-4/70 computer.

(iii) The laboratories, and graduate manpower available for neutron nuclear data work in the United Kingdom are presented in Table 2.3. In assessing the evaluation effort we have included data library maintenance work (format manipulations, checking, editing and so on), and associated computer programming; on the other hand we have attempted to discriminate against

(a) An experimenter's normal level of work on the analysis of his own measurements.

(b) Derivation of multigroup cross-sections, testing against complex integral data, and related data "adjustment" work.

The committees and working parties involved in the organisation of the national neutron nuclear data measurement and evaluation programme have been briefly described in section 1 above. The organisational scheme, is approximately as shown in Table 2.4.

(iv) The UK Atomic Energy Authority has played an active role in promoting co-operation between evaluators. A loose measure of multi-national co-operation has been achieved between the ENEA member countries through meetings of the EANDC-EACRP Joint Sub-Committee on Nuclear Data Evaluation. This has initiated in Europe the series of Neutron Nuclear Data Evaluation Newsletters which has been very successfully organised and edited by Ribon at Saclay. The United Kingdom makes regular contributions to this newsletter.

The Joint Sub-Committee has also been instrumental in promoting the exchange of evaluated data files between OECD member countries through the data centres at Saclay and Brookhaven. The current interest of the Joint Sub-Committee is to explore whether a closer co-ordination of evaluation efforts can be usefully and effectively promoted, especially in Europe, perhaps through small specialist meetings on specific topics. It is too early to say what the outcome will be.

TABLE 1.1

Evaluations needed for the UK reactor programme: a brief review of the relevant data files

Material	DFN	Comments
H	901	Adequate - H in H_2O; could be improved marginally.
D	905	Recently revised - D in D_2O.
He^3	220D	Believed adequate. ENDF/B file MAT-1088 may be marginally better for natural He and is being converted to UKNDL format.
He^4	221D	
Li^6	214D	An old file; revision in progress.
Li^7	215D	An old file; probably adequate for the present.
Be^9	50A	Reasonably satisfactory, but virtually no requirement.
B^{10}	90A	A new file.
B^{11}	49A	Probably adequate, but could be improved.
C	902A	A new file.
N	259	Probably adequate, but could be improved.
O	33D	Believed adequate - mainly ENDF/B MAT-1013; LASL revision above 6 MeV to be incorporated in due course.
Na^{23}	(93)*	ENDF/B file MAT-1059 converted to UKNDL format and is probably adequate for the present.
Mg	-	Not required and no complete file available.
Al^{27}	35E	Probably adequate - revision desirable, especially σ_γ in the resonance range.
Si	25D	Very old file - σ_γ needs improvement in the resonance range.
Cl	141D	Very old file.
Cl^{37}	( )	Preliminary new file - improvements needed for p-wave neutron capture.
K	84A	Probably adequate for the present - mainly GA file MAT-5005.
Ca	138D	Very old file.
Ti	190A	May be adequate - mainly UNC evaluation. The new ENDF/B file should be better but further revision in the resonance range may be needed, especially σ_γ.

*Useable, but some format corrections still in progress.

Material	DFN	Comments
V	(952)	ENDF/B file MAT-1017 being converted to UKNDL format and may be adequate - but see comments for Ti.
Cr	45D	Elderly file of French origin available; revision is needed, especially of σ_γ in resonance range.
Mn^{55}	(88)*	ENDF/B file MAT-1019 converted to UKNDL format and believed adequate.
Fe	(906)	Newly revised in resonance range. ENDF/B file MAT-1124 is being converted to UKNDL format and will be used above 330 keV.
Co^{59}	235A	Capture cross-section only - an old file; no requirement however.
Ni	(907)	Revision nearly complete in resonance range. ENDF/B file MAT-1123 is being converted to UKNDL format and will be used above 240 keV.
Cu	73	Probably adequate.
Ga	105A	Very old file; may be adequate but revision in the resonance range is desirable, especially σ_γ.
Zr	82A	Probably adequate; could be further improved in the resonance region.
Nb	79A	Mainly ENDF/B file MAT-1024; probably adequate but MAT-1112 may be better.
Mo	81A	Mainly ENDF/B file MAT-1025. Revision of fast neutron cross-section is in progress, but revision in the resonance range is needed also - especially σ_γ.
Cd Cd^{113}	70) 71A)	Recent compilations, believed adequate.
Xe^{135}	4E	Believed adequate - extends to 1 keV only. DFN-750, giving σ_γ only from 0.0001 eV to 10 MeV, needs revision.
Ta^{181}	328A	Believed adequate.
W	213A	Probably adequate.
Au^{197}	222D	Complete revision of σ_γ desirable, especially in resonance range, as reference standard; but no reactor requirement. ENDF/B file MAT-1037 might be a better basis for such a revision.
Pb	26B	Very old file, probably adequate.

*Useable, but some format corrections still in progress.

Material	DFN	Comments
Th^{232}	22A	Very old file - complete revision desirable. For fission cross-section only, DFN-332 is preferred.
Pa^{233}	86	May be adequate.
U^{233}	87A	A fairly new file, adequate for the present.
U^{234}	74A	Covers range 1 keV to 15 MeV only. Conversion of ENDF/B file MAT-1043 proposed.
U^{235}	271A	Recently revised above 25.5 keV, using older file DFN-66A at lower energies; nu-bar revised over whole energy range. A GENEX file spanning the range 0.4 eV to 25 keV is available also; it is more up-to-date than DFN-66A and is being further revised.
U^{236}	75A	Covers range 1 keV to 15 MeV only. Conversion of ENDF/B file MAT-1046 proposed.
U^{238}	272	Recently revised above 25 keV; using at lower energies older French file DFN-401A. A new GENEX file is available also spanning the range 0.4 eV to 25 keV after a detailed review, especially of σ_γ.
Np^{237}	61	Fission cross-section file; needs revision especially in resonance range. The new ENDF/B file would probably be the best basis for such a revision.
Pu^{238}	216D	May be adequate for the present.
Pu^{239}	269A	Recently revised above 8.5 keV, using older file DFN-65A at lower energies; nu-bar revised over whole energy range. The new French file DFN-404A is also available and graphical comparisons are in progress. A new GENEX file is available also from 0.4 eV to 25 keV.
Pu^{240}	402A	New French data file; probably adequate.
Pu^{241}	403A	New French data file; probably adequate.
Pu^{242}	(953)	The ENDF/B file MAT-1055 is being converted to the UKNDL format and will probably be adequate.
Am^{241}	(954)	See comment for Pu242; MAT-1056 being converted.
Am^{242m}	-	Long term requirement; no file available.
Am^{243}	(955)	See comment for Pu242; MAT-1057 being converted.

Material	DFN	Comments
Cm^{242}	-	Long term requirement.
Cm^{244}	(956)	See comment for Pu242; MAT-1058 being converted.
Fission products	701-778	Files of capture cross-section data are available and may be adequate, but revisions are desirable especially in the resolved resonance range and representative scattering data are needed for bulk fission products. New capture cross-section files have been compiled recently for Kr^{83} (DFN-904) and Pm^{147} (DFN-903).

TABLE 2.1

Work in progress and aspirations for the remainder of 1971

Material	Reactions	Comments
He (II)	(n,n) (n,p)	ENDF/B file MAT-1088 to be converted to UKNDL format: Hammond (AEEW).
Li^6 (I)	All; esp. (n,n) (n,t)	Uttley (AERE) has reviewed cross-sections and elastic angular distributions below 500 keV. Uttley & Sowerby (AERE) are extending the evaluation to 5 MeV.
C (II)	TSL	Investigation of effect of anisotropy of graphite crystals on thermal scattering law: Butland (AEEW).
Na^{23} (II)	All	Existing conversion of ENDF/B file MAT-1059 to UKNDL format (DFN-93) does not yet satisfy all usual format conventions, and is to be regenerated: Pope (AEEW).
Mg (II)	All	First steps have been taken in conversion of ENDF/B file MAT-5002 to UKNDL format - very low priority; Pope (AEEW).
V (I)	All	ENDF/B file MAT-1017 converted to UKNDL (DFN-952), but many format corrections needed; Hammond (AEEW).
Mn^{55} (II)	All	Conversion of ENDF/B file MAT-1019 to UKNDL format does not yet satisfy all usual format conventions, and is to be regenerated; Pope (AEEW).
Cr (I)	(n,n) (n,γ)	Evaluation in resonance range has been started; (Moxon (AERE).
Fe (I)	All	Newly revised in resonance range (DFN-906). ENDF/B file MAT-1124 converted to UKNDL format for use above 330 keV, but many format corrections still needed, and modification of the representation of inelastic-to-continuum secondary neutron energy distribution: Hammond & Spanton (AEEW).
Ni (I)	All	Revision nearly complete in resonance range as DFN-907: Moxon (AERE) and Pope (AEEW). ENDF/B file MAT-1123 is being converted to UKNDL format for use above 240 keV; Hammond (AEEW). The (n,α) cross-section is under review by Douglas (AWRE).
Nb^{93} (II)	All	Conversion of ENDF/B file MAT-1112 to UKNDL format may be attempted.
Mo (I)	(n,n) (n,n') (n,α)	Evaluation in progress in fast neutron energy range; Douglas (AWRE)

Material	Reactions	Comments
Th^{232}	All	Conversion of ENDF/B file MAT-1117 to the UKNDL format may be attempted, with low priority.
U235	(n,f)	GENEX file to be forced into agreement with "simultaneous fit" in the range 0.1 eV to 25 keV; Macdougall (AEEW).
U234	All	Conversion of ENDF/B files MAT-1043, -1046, -1055, -1056, -1057, -1058 to UKNDL format has been started; Cameron (AWRE), Dean & Hammond (AEEW).
U236	"	
Pu242	"	
Am241	"	
Am243	"	
Cm244	"	

TABLE 2.2

Computer facilities and programmes used for evaluation work and for handling evaluated data libraries

A) The following computers are used for these purposes:

At Aldermaston: IBM-360/75; an IBM-2250 CRT console is linked to this computer. A Ferranti Atlas computer is also available, and is sometimes used by evaluators to generate input for a CRT plotter.

At Harwell: IBM-360/75; a Calcomp CRT plotter is available.

At Winfrith: KDF-9 and ICL-4/70; an IBM-360/30 is also used for tape copying and mode conversions, and to provide a link with the Harwell computer.

B) The UKNDL is the principal nuclear data library in use in the United Kingdom. The format has been described by Parker in AWRE O-70/63, and the last published summary of the contents is that of Norton AEEW-M 824 (1968); Table 1.1 gives some indication of recent additions.

The GENEX data library contains tapes of resonance cross-section data in very great detail (about 120,000 energy points) over the range 0.4 eV to 25 keV for a few fissile and fertile materials U235, U238, Pu239, Pu240 and Pu241. The data are represented in a binary format; see for example Brissenden & Durston AEEW-R 622 (1968).

C.1) Following are brief details of the principal computer programmes used for manipulation of evaluated data.

Programme	Language	Computer	Purpose
LCHECK	Egtran-2*	KDF-9	Reads cards to tape with elementary sequential check.
CHECK-1	Fortran-4≠	IBM-360/75	Checks format and arithmetical consistency of data files.
CHECK-2	Fortran-2	KDF-9	
AMEND	Egtran-2	KDF-9	) For amending and modifying
JACKDAW	"	"	) data files in various
GRAFT-3	"	"	) ways.
EDIT	Egtran-2	KDF-9	For merging files from various tapes to form a data library.
MINIGAL	Egtran-2	KDF-9	Computes resonances integrals and fission-spectrum averaged cross-sections from a data file.
GROD	Fortran-4	IBM-360/75	Prepares tapes for graphical representation of Data using a CRT plotter.
PANDIT	Fortran-4≠	IBM-360/75	For adjusting UKNDL data files from calculated adjustments to group cross-sections.≠≠
GALAXY	Egtran-2	KDF-9	Principal users' programme for computing multigroup cross-sections from UKNDL.
	Fortran-4≠	IBM-360/75	

* Egtran-2 is a dialect of Fortran-2 developed for the KDF-9 computers.

≠ Conversion of these programmes to Fortran-4 is in progress.

≠≠ It should be emphasised that adjustments of this kind have not been made to any of the basic data files in the UKNDL.

2) Following are brief details of some of the principal computer programmes used for analysis and calculation of neutron cross-sections:

Programme	Language	Computer	Purpose
LEAP	Fortran-4	ICL-4/70	Calculate thermal scattering law from phonon frequency function, in incoherent model.
SLAB	"	"	
TOR	"	"	
PIXSE	Egtran-2	KDF-9	Calculate thermal inelastic cross-sections from scattering law.
	Fortran-4	ICL-4/70	
SOLON	Fortran-4	ICL-4/70	
GIEN	"	"	
HEXCOH	Egtran-2	KDF-9	Calculates coherent elastic scattering of monatomic hexagonal crystals.
SIGAR	Egtran-2	KDF-9	Calculates σ_T, σ_n, σ_γ in multi-level Breit-Wigner formalism, for $l = 0$ to 5. Doppler broadened output in UKNDL format.
REMO	Egtran-2	KDF-9	Calculates σ_T, σ_n, σ_γ, σ_F by Reich-Moore method, for $l = 0$ only. Provides input to TEMPO.
TEMPO	Egtran-2	KDF-9	Doppler broadening of arbitrary cross-sections with output in UKNDL format.
MLCSC	Fortran-4	IBM-360/75	Multi-Level Cross-section Calculation in R-matrix formalism for $l = 0$ to 3, with Doppler broadening. Gives σ_T, σ_n, σ_γ, but not in UKNDL format.
- - -	Fortran-4	IBM-360/75	Similar to MLCSC, includes σ_F, for $l = 0$ only.
SIGAV	Egtran-2	KDF-9	Calculates averaged σ_T, σ_n, σ_γ from resonance statistical parameters, for $l = 0$ to 4. at present only for spin 0 target nuclides.
CWF	Egtran-2	KDF-9	Calculates Coulomb penetration and shift factor, for $l = 0$ to 5.
OPW	S-2≠	IBM-7030	Optical model; includes a fast search routine for parameter fitting.
HFW	S-2≠	IBM-7030	Hauser-Feshbach calculations, with option for Moldauer correction.
SCORE	Fortran-4	IBM-360/75	Uses IBM-2250 CRT console for computer-interactive-graphic display of NEUDADA and ENDF/B data files with output in UKNDL format.

≠ S-2 is a dialect of Fortran-2 developed for the old IBM-7030 computer. The programmes OPW and HFW have probably been converted to Fortran-4 for the IBM-360/75.

C.3) A programme for conversion of ENDF/B files to UKNDL format has recently been developed by Cameron (AWRE), in Fortran-4 for the IBM-360/75 computers; it is now being tested in use.

The programme SCATTER written in Egtran-2 for the KDF-9 computer, generates normalised tabular angular distributions in the centre-of-mass frame, from Legendre polynomial series representations in either frame. Output is in UKNDL format.

Various programmes have been written ad hoc, from time-to-time, for piece-meal conversions from SPENG, KEDAK, ENDF/B, and other formats into the UKNDL format.

TABLE 2.3

Laboratories involved in neutron nuclear data evaluation, and the graduate manpower involved

Laboratory	Graduate manpower for evaluation
AEE, Winfrith	About 50 man months in 1971 Perhaps 40 man months in 1972
AERE, Harwell	About 30 man months in 1971 Perhaps 20 man months in 1972
AWRE, Aldermaston	About 36 man months in 1971 Perhaps 7 man months in 1972

APPLICATION OF EVALUATED NUCLEAR DATA FILES AVAILABLE AT IAEA FOR REACTOR CALCULATIONS

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Abstract

A program system has been developed for handling of evaluated data files KEDAK and UKAEA and for calculation of multigroup constants from them. Method of production of reactor group constant libraries is discussed and some test calculations are presented.

1. Introduction

The recent development of reactor calculations in our country [1] has required a reliable set of group constants. In the published literature there can be found some sets of microgroup constants, as e.g. [2] , [3], etc. These constants have been produced from evaluated nuclear data which originally resulted from nuclear theory and experiments. The group constants sets have been published over a relatively long period of time and they are not flexible enough as far as the calculation methods and special cicumstances are concerned, e.g. diffusion, transport and Monte Carlo calculation, heterogeneous systems, shielding calculations, etc.

Recently, evaluated data of some isotopes which are important in reactor physics have become available at IAEA on magnetic tape file. It is hoped that in the future the accuracy of the nuclear data and the assortment of material available at IAEA will grow, thereby satisfying requirements concerned with the group constants in reactor physics calculations.

In order to make use of the IAEA nuclear data service a system of programs has been developed for the ICL-1905 computer to produce multigroup constants for reactor and shielding calculations. The main programs of this system are: PRODGROUP, ZEBRA-I, ZEBRA-2. Besides these programs, there are smaller programs for data tape testing, library editing, and so on.

2. The PRODGROUP program

PRODGROUP program [4] is composed of three stages connected to each other by magnetic tape interface. The most important is the first stage producing the DF1 interface magnetic tape file. DF1 contains fifteen data types for each element in strict order and format. An effort has been made to render DF1 independent of the source of evaluated data, i.e. the form of the data sets of any element on DF1 should not on whether KEDAK or UKAEA data have been used. This and the strict order of data types render the DF1 a very convonient starting point for any further calculation.

The second stage of PRODGROUP produces DF2, which can be considered as a library tape for multigroup macro-constant calculations. The cross-sections are stored on DF2 so that the energy argument corresponds to an ultrafine-mesh energy-group system. This system is independent of elements.

The third stage of PRODGROUP produces shielded multigroup macroconstants for mixtures of elements by making use of DF2.

The second and third stage of PRODGROUP are mathematically tested, however they have not yet been used for practical purposes because a calculation with satisfactory accuracy requires too much computing time on our computing facility.

3. ZEBRA-I program

ZEBRA-I [5] produces a MUFT-type forty-group constant library from DF1. This library can be directly used by the program GRACE [6], which is a multigroup fast neutron spectrum code. GRACE

calculates few-group macroconstants for 2-D diffusion calculations by the code SYSIPHUS [7].

The constants produced by ZEBRA-I are used above the thermal region, except in the resonance region of heavy elements. The resonance integrals for heavy elements in a cylindrical cell and in homogeneous mixtures can either be calculated by the programs RIFFRAFF and RA04 [8]., respectively, or by the so-called BIGG-type resonance treatment, which is a semiempirical method. RIFFRAFF and RA04 make use of the resonance parameters of heavy elements /U^{235}, U^{238}, Pu^{239}/ given in the KEDAK data.

In order to test our library, we have recalculated the results of NORA critical experiments [9] /see Table/*.

4. ZEBRA-2 program

The program ZEBRA-2 produces multigroup constant sets /up to 26 groups/ for the program MUSHPALB [10], which calculates the spectrum of neutrons transmitted through multilayer shielding. ZEBRA-2 also starts out from DF1 the finel product of its job being a library tape whose format is the same as that originally produced from ABBN data [11] [12].

ZEBRA-2 mainly based on ZEBRA-I. The difference is in the calculation of the elastic transfer matrix, which has been taken over from PRODGROUP [4].

Testing of ZEBRA-2 is in progress. A preliminary result is shown on the figure. The experimental curves are taken from [13].

5. Evaluated nuclear data and integral nuclear data requirements

Most users of nuclear data in the field of reactor physics require integral quantities derived from cross-section

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*Recently an error has been detected in GRACE. This is why our results differ slightly from those reported in [5].

curves rather than the cross-section curves themselves. By the term "integral quantities" we mean here:

a/ Multigroup constants for general reactor calculation

b/ Removal cross-sections and other constants for shielding calculation.

c/ Spectrum-integrated activation cross-sections for experimental reactor physics and isotopic production

d/ Spectrum-integrated activation cross-sections for activation analysis.

These integral nuclear data can, of course, be obtained from evaluated nuclear data by means of standard computing techniques. However the transporting of the enormous quantity of nuclear data is often inconvenient and their handling requires a special program system which is not available everywhere. This is why it would be desirable that the nuclear data centers, and above all the Nuclear Data Section of IAEA, could undertake the job of producing at least a part of the integral data requested by the users. The staff of our laboratory - within the limit of our possibilities - is ready to assist the Nuclear Data Section in this work.

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Comparison with NORA experiments

Case No.	B_m^2 /m^{-2}/			Q^{28}			δ^{25}		
	exp.	calculated in [7]	calculated by us	exp.	calculated in [7]	calculated by us	exp.	calculated in [7]	calculated by us
1	12.43±1.2	11.05	11.1	0.374	0.315	0.389			0.0190
2	17.74±0.26	17.16	17.2		0.709	0.857			0.0414
3	20.1±0.2	19.38	19.2	1.292	1.250	1.50			0.0726
4	19.93±0.24	17.76	16.7	2.205	2.32	2.75			0.135
5	16.87±0.55	15.54	13.8	2.893	3.00	3.52			0.175
8	33.21±0.47	27.9	30.5	1.035	1.058	1.19	0.069	0.063	0.057
9	36.65±0.41	30.89	33.1	1.308	1.438	1.61	0.100	0.086	0.0783
10	33.93±0.4	30.03	30.8	1.992	2.230	2.48	0.153	0.134	0.122
11	29.91±0.32	24.91	23.5	2.865	3.23	3.57	0.183	0.198	0.180
13	37.7±0.65	30.14	35.0	0.778	0.889	0.982	0.057	0.053	0.047
14	49.98±0.43	42.11	46.5	1.218	1.330	1.46	0.080	0.079	0.709
15	51.89±0.7	44.00	46.7	1.77	1.880	2.05	0.105	0.113	0.101
16	40.47±0.31	35.26	34.0	2.717	3.24	3.49	0.208	0.199	0.176

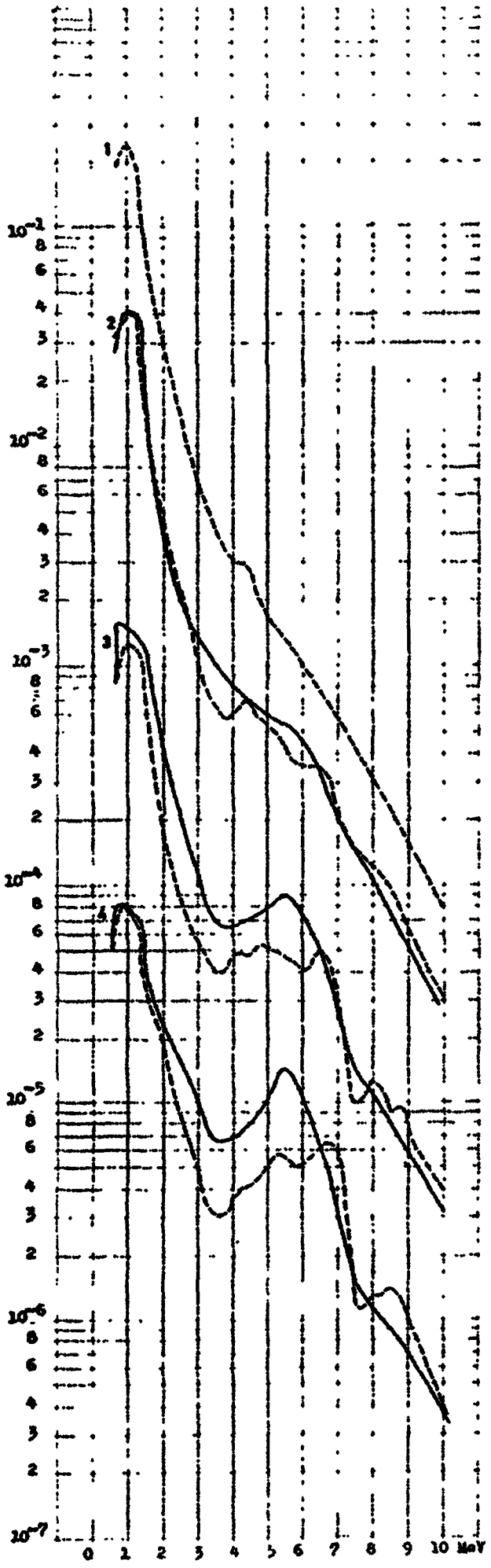

Fig.1 - Fast neutron spectra transmitted through graphite layers
1 - source spectrum, 2, 3, 4 - spectra of neutrons transmitted through graphite of thickness 12, 36, and 60 cm, respectively
——— spectra, calculated by us
- - - - measured spectra taken from [13] /Fig. 7/

REVIEW OF NUCLEAR DATA WORK FOR REACTORS IN INDIA

by

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A B S T R A C T

This paper reviews the nuclear data work done in India in connection with the Indian Nuclear Power Programme. The work done on data evaluation and preparation of multigroup cross section libraries has been discussed. Some of the difficulties experienced in the adaptation of evaluated nuclear data libraries are also discussed. A specific suggestion has also been made to the Agency's NDS to obtain and make available a few multigroup cross section sets.

INTRODUCTION

The Indian Nuclear Power Programme is based mainly on heavy water moderated reactors in the first stage and fast breeder reactors in the second stage. Of the first category, two units of 200 MW(e) each are in the final stages of construction while two other stations of same capacity are in the initial stages. A 500 MW(e) system in the same category is in the planning stages. Towards the development of fast reactors, it is proposed to build a 40 MW(th) Fast Breeder Test Reactor and a Fast Pulsed Reactor and its associated critical facility the latter one intended mainly for Physics experiments. The Reactor Engineering Division of Bhabha Atomic Research Centre has been entrusted with the responsibility of detailed physics design of the afore mentioned reactor concepts and this naturally led to the evaluation of nuclear data for the materials of interest in our programme. The following paragraphs present the work done in this direction.

EVALUATION OF CROSS SECTIONS

Because of the limited experimental facilities, there has been no contribution to the evaluation of energy point cross-sections from experiments. However, we undertook theoretical evaluation of point cross-sections for certain materials in the energy range 0.1 MeV to 10 MeV. The materials evaluated were Cr, Fe, Ni-58, Ni-60, Mo, Cd, Pb, Th, U-235, U-238 and Pu-239 for total, elastic and inelastic scattering cross-sections. These cross-sections were not stored as evaluated data libraries but were immediately used to generate group cross-sections for multigroup schemes for neutronic analysis of fast reactors.

To supplement our work we have acquired ENDF/B from U.S.A, and KEDAK and U.K.Nuclear Data Libraries through the courtesy of IAEA. However, adaptation of these libraries and their associated data processing codes has encountered some difficultics because of the limited computer memory at our disposal (32 K of CDC-3600). We would very much appreciate sharing the experiences of other member countries in this direction. Moreover, exchange of these and other evaluated data libraries involves some technial difficulties also mainly in that only seven track tapes can be read by CDC-3600.

EVALUATION OF GROUP CROSS SECTIONS

Consequent on the difficulties met with in the adaptation of evaluated data libraries, we are concentrating more on the preparation of multigroup cross-section libraries and modification of the existing ones. To this end following work has been done:

a. A 26-group cross-section set with the weighting spectrum of a typical large fast power reactor has been generated with particular emphasis on resonance region. The latest evaluation of σ_c for U-238 and α for Pu-239 have been recently incorporated to update the cross-sections for these materials.

b. The 26-group Russian set has been extensively modified in view of the recent data generated by experimentalists and evaluators. In particular, the group fission cross-sections of Th-232, U-233, U-234, U-235, U-236, Np-237, U-238, Pu-239, Pu-240, Pu-241 and Pu-242 and capture cross-sections for Mo, U-238 and Pu-239 have been regenerated.

c. For the physics calculation of Fast Breeder Test Reactor the 25-group Cadarache Version II library is used. Thorium self-shielding factors in this library have been modified based on the latest resonance parameters.

d. For thermal reactor calculations, a 26-group library in the fast and resonance energy ranges is being developed. Group resonance integrals as functions of background cross-section and temperature for U-238 have been generated with resonance parameters from Schmidt and BNL-325. It is planned to supplement this with Th-232, U-233, U-235 and Pu-239. Also available at present are the group cross-sections for H-1, D-2, O-16, Al-27 and Zr based on MUFT cross-sections. It is also intended to cross-check the resonance group cross-sections using parameters from ENDF/B, KEDAK and UK Nuclear Data Libraries.

REQUIREMENTS

The recently measured and evaluated cross-section data for light elements (Na, Cr, Fe, Ni and Cu), and heavy elements (Th-232, U-233, U-234, U-235, U-236, U-238, Pu-239, Pu-240, Pu-241 and Pu-242) along with their recommended resonance parameters are required for the correct prediction of neutronic characteristics of fast reactors. As we have initiated preliminary studies on MSBR, updated data for Li-7 and F-19 are also needed.

CONCLUSION

In view of the problems faced in the adaptation of evaluated nuclear data libraries arising from the computer at our disposal, preparation of multigroup cross-section sets assumes a greater importance for the prediction of physics performance of fast and thermal reactors. To check the suitability and correctness of the cross-section sets generated by us, inter-comparison of our predictions with those from other available libraries is highly desirable. We would, therefore, like to make a specific request to the Agency to use their good offices to make available to us the updated multigroup cross-section sets like WIMS, GAM, METHUSELAH and SNEAK Modified 26-Group Set. These would in fact render more help than the evaluated point cross-section libraries.

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"Neutron Nuclear Data Evaluation Activities in Japan "

by

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Abstract

This is a brief description of the neutron nuclear data evaluation activities in Japan, as of August 1971. As an example, the evaluation work on fission product data is briefly introduced here.

Works on neutron nuclear data in Japan have been performed under coordination of JNDC (Japanese Nuclear Data Committee). JNDC organizes two working groups in order to find solutions of existing problems on the nuclear data. One of the two working groups is Reactor Constants Working-Group, in which the members engage in investigating the problems on the reactor constants. The other working group is Nuclear Data Working-Group, in which the members collect and review the nuclear data obtained experimentally. Works on the evaluation of the nuclear data in JNDC are performed by some members of the Nuclear Data Working-Group.

Some works on compilation and review of neutron nuclear data have been completed recently. As mentioned in Neutron Nuclear Data Evaluation Newsletter, compilations of neutron elastic and inelastic scattering cross-section data of Na and O have been finished in the energy region of 10 keV to 15 MeV. Report on compilation and review of the data for ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu will be published in the near future. Numerical data used in these works have been collected mainly from NEUDADA files by the request to CCDN, and the other data have been obtained by surveying published reports.

Evaluation of the total neutron cross section of carbon up to 2 MeV and evaluation of $^{27}Al(n,\alpha)$, $^{56}Fe(n,p)$, $^{63}Cu(n,2n)$, $^{65}Cu(n,2n)$ from thresholds to 20 MeV have been completed, and the reports of these works are now in the press.

In JNDC, there are some programs on the neutron nuclear Data evaluation. These are evaluations for ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu, ^{233}Pa, ^{239}Np and fission products. As an example of evaluation activity in JNDC, evaluation on fission product data is briefly introduced here. After surveying decay-chain of fission products and the life-times, 177 nuclei are selected as the important nuclei. These consist of 142 nuclei selected by Benzi et al. and additional 35 nuclei. Experimental data for the 177 nuclei are collected by the request to CCDN and by surveying published literatures. In this work, quantities studied mainly are fission product yields, neutron capture cross-sections and inelastic scattering cross-sections.

In the mass region of the fission products, there are many nuclei of which data are not measured yet. Therefore, it is necessary to look for some possible systematics of the data on mass number and/or on the incident neutron energy. For fission product yields, calculations are performed by using computer program STAF, and results of the calculations are compared with the experimental data to look for the above mentioned systematics.

Neutron capture cross-sections evaluated by Benzi et al. are adopted in the present work. Systematics of the neutron capture cross-sections are studied based on Benzi's evaluated data and existing experimental data. Calculations are also performed by using the computer code RACY, in order to survey some possible trends of the parameters involved in the computer code.

To obtain the inelastic scattering cross-section, many calculations are needed, since there are scarcely any experimental data available in the mass region of the fission products. The optical potential parameters

are required in order to estimate the inelastic scattering cross-section. The systematic trend of the optical potential parameters are searched for by fitting the total cross-sections of several nuclei. The calculations are performed by using computer code TOTAL. These works are now in progress.

NUCLEAR DATA ACTIVITIES IN ROMANIA

by

S.Râpeanu

Abstract

The paper briefly reviews the measurement and evaluation activities in the field of neutron data in Romania with special emphasis being given to the generation of multigroup constants from evaluated data libraries.

The present demands of nuclear energy in Romania [illegible] setting up libraries of nuclear data and group constants for reactor calculations.

Nowadays, the activity in this field is perfoming on within three groups, under the general supervision of the SCNE (State Committee for Nuclear Energy) :

a) a group whose task is to set up the nuclear data library; this group has carried out a general study on the present status of evaluated data available in several centers as well as on the methods of obtaining and storing the nuclear data in our own library. At the same time, this group is also involved in problems of evaluation and compilation.

b) a second group is involved in nuclear physics, both experimentally and theoretically. Further details on its activity can be found out in Annual Report - INDC (RUM-2/G), compiled by dr.A.Berinde. From this, worth mentioning is the work "Absolute measurement of Pu^{239} fission cross-section", performed under the research contract RB-422, sponsored by the IAEA. There could be also mentioned the works of some cross-sections evaluations for S^{32}, Ni^{60} Fe, Cr, As^{75}, Ca, Ta in the range 1 KeV-15 MeV as well as certain computer codes in this field.

This group has at its disposal the following facilities :

- a research reactor VVRS
- a few subcritical assemblies
- a cyclotron U-120
- a betatron of 25 MeV of our own construction

- a significant contribution will be brought by the accelerator Van der Graaf tandem FN-15
- a lot of auxiliary devices, of which we mention the multichannel analyser with 4o96 channels.

c) a third group involved in the creation of a group constants library to meet our specifical demands. This group has been founded at the end of 1971 and carries on its activity within the Institute for Nuclear Tehnology (ITN), whereas the first two groups belong to the Institute for Atomic Physics.

Because of the handling difficulties of a data library the activity aiming to create sets of group constants will not be able, in the first stages, to rely on a nuclear data library. In the further stages we think necessarily that our own data library should have codes for the automatization of group constants production as well as codes for internal check up, by means of self-consistency controls and comparison with integral experiments.

A sharp question is the possibility to obtain some nuclear data libraries.and the possibility of an international cooperation. There arises rather often the question whether a data library may be a matter of free exchange; in our opinion a data library is a matter ofnuclear physics, even if its final task is an applied one.

As to the computing codes it often arises the situation that starting up from the same physical theory, say the same mathematical formulae, the results obtained in several countries with several codes are dissimilar. The initiative of IAEA to list and compare the codes is very valuable. However, the nuclear research centers from different countries could coordinate their plans in order to avoid parallel work. Surely, one cannot completely avoid the parallel work but it is worth diminishing it.

Alike the previous cases it appears necessary that IAEA should stimulate the listing of group constants sets presently existent and assure their free exchange. To the same effect it appears necessary to analyze each such a set of group constants by means of comparison with similar sets and integral experiments. The discrepancies between the group constants obtained on the basis of the same data library should be analyzed and, starting from this analysis, recommendations on how to calculate the group constants should be made. To this aim the creation of working groups is to be recommen-

ded. The conclusions of these working groups could be gathered within a reactor group constants handbook, whose usefulness is obvious.

I should like once again to underline the valuable efforts of the NDS-IAEA, to achieve a broad international cooperation in this field of activity.

АВТОМАТИЗАЦИЯ ПРОЦЕССА ПРОВЕРКИ ИНФОРМАЦИИ ДЛЯ БИБЛИОТЕКИ РЕКОМЕНДОВАННЫХ ЯДЕРНЫХ ДАННЫХ, ПРОГРАММА ПОСОШОК

В.Е. Колесов, А.С. Кривцов, Н.А. Соловьев

А Н Н О Т А Ц И Я

Описывается Программа Обнаружения Случайных ОШибОК (ПОСОШОК), составленная на языке АЛГОЛ-60 применительно к вычислительным машинам типа М-220. Программа ПОСОШОК предназначена для проверки правильности представления и самосогласованности числовой информации, содержащейся в Библиотеке рекомендованных ядерных данных ФЭИ.

В процессе работы программа ПОСОШОК проверяет:

I) правильность нумерации перфокарт в секции и секций в файле;

2) соответствие информации, включенной в нулевую секцию, заголовкам и фактическому содержанию последующих секций файла;

3) согласованность между различного рода заголовками и фактическим содержанием массивов данных внутри секции, которым эти заголовки предпосланы;

4) допустимость значений для тех или других величин, исходя из их физической природы или способа определения;

5) упорядоченность данных в пределах некоторого массива;

6) непротиворечивость друг другу различных величин, если они связаны между собой определенной зависимостью;

7) правильность нормировки угловых распределений и энергетических спектров вторичных нейтронов;

8) плавность хода нейтронных сечений и специальных величин, заданных в виде детальной энергетической зависимости (проверка на "выбросы").

Все обнаруженные в результате этих проверок ошибки и несоответствия выдаются на печать в стандартном кодированном виде.

Описываемый здесь вариант программы имеет дело со следующими классами ядерно-физических данных:

а) нейтронные сечения,

о) угловые распределения вторичных частиц,

в) энергетические распределения вторичных частиц,

г) специальные величины для нейтронов

I. Введение

Для расчетов ядерных реакторов требуется большое количество разнообразных данных, характеризующих взаимодействие нейтронов и гамма-квантов с ядрами топливных элементов, замедлителей и конструкционных материалов. Возникает настоятельная потребность накапливать и хранить такого рода данные с тем, чтобы затем использовать их в расчетах. Для этих целей создаются специальные машинные библиотеки рекомендованных ядерных данных [1].

Такие библиотеки существенно расширяют возможности подготовки исходной информации для реакторно-физических расчетов. Они позволяют в значительной степени автоматизировать процесс переработки рекомендованных ядерных данных в групповые константы с произвольным энергетическим разбиением и, таким образом, дают возможность непосредственно связать этот процесс с процессом расчета ядерных реакторов в рамках метода групп.

Нейтронные сечения и другие ядерно-физические данные, рекомендованные для расчетов ядерных реакторов, хранятся на перфокартах и магнитных лентах в стандартном представлении, удобном для обработки этих данных на ЭВМ. Описание общей структуры и форматов библиотеки ядерных данных, принятых в Физико-энергетическом институте, содержится в работе [2].

С библиотекой рекомендованных ядерных данных связан целый комплекс программ различного назначения. Сюда относятся:

- программы, использующиеся для создания самой библиотеки рекомендованных ядерных данных и поддержания ее в рабочем состоянии, и
- разного рода обрабатывающие программы, которые при своей работе используют данные, хранящиеся в библиотеке ядерных данных.

В данной работе описывается Программа Обнаружения Случайных ОШибОК (ПОССОШОК), составленная на языке АЛГОЛ-60 применительно к вычислительным машинам типа М-220. Программа ПОСОШОК предназначена для проверки правильности представления и самосогласованности числовой информации, содержащейся в Библиотеке рекомендованных ядерных данных ФЭИ.

Авторы считают своим долгом выразить искреннюю признательность В.Г.Золотухину и М.Н.Николаеву за неизменный интерес и внимание к настоящей работе на всех стадиях ее выполнения.

2. Общая характеристика программы ПОСОШОК

Перед тем как включить в библиотеку некоторые новые ядерно-физические данные и тем самым ввести их в постоянное употребление, следует

Note An English translation of this paper is available, upon request from the IAEA Nuclear Data Section, as document INDC(CCP)-23/G.

убедиться в правильности их представления на первичных носителях, какими обычно являются перфокарты. При большом объеме данных, когда в обращение включается значительное количество перфокарт, нельзя игнорировать вероятность появления случайных ошибок, связанных с разного рода переписками, набивкой и т.д. В таких случаях проверка правильности представления данных на перфокартах приобретает особую актуальность.

Надежная проверка правильности набивок может быть обеспечена путем непосредственного сравнения содержания набитых карт с листами, по которым производилась набивка данных на перфокарты. Но при большом объеме информации практическая реализация такой проверки представляет собой трудную задачу, поскольку визуальная проверка перфокарт или полученных с них печатных таблиц является чрезвычайно трудоемкой и утомительной процедурой. Проверку данных однако можно производить с помощью ЭВМ, используя для этих целей специальные программы.

Программа ПОСОШОК представляет из себя такого рода программу, предназначенную для проверки библиотечных данных. Она позволяет в значительной степени автоматизировать и тем самым существенно облегчить процесс проверки представления информации на перфокартах или магнитной ленте. Анализируя данные, представленные в библиотечном формате, программа производит над ними большое число разного рода логических и арифметических проверок. Все обнаруженные в результате этих действий ошибки и несоответствия выдаются на печать в стандартном кодированном виде.

Машинная проверка данных заслуживает внимания несмотря на то, что требует включения в библиотеку в некотором смысле излишней или повторяющейся информации. Такая проверка оказывается полезной и, как правило, эффективной.

Программа проверки рекомендованных ядерных данных в процессе работы имеет дело с огромными массивами данных, достигающими в настоящее время объема 40-50 тысяч чисел для одного ядра определенного сорта. К тому же сама программа, ввиду логической сложности и значительного числа проводимых проверок, имеет большой объем и занимает в памяти машины много места. Все это накладывает определенные требования на программу и вычислительную машину, на которой данная программа работает. Решающую роль при этом начинает играть объем оперативной машинной памяти, а также развитость системы внешних запоминающих устройств (магнитные барабаны, диски, магнитные ленты и др.)

Оптимальная организация процесса проверки библиотечной информации требует для своей реализации ЭВМ с большой оперативной памятью для того, чтобы в течение всего периода работы программы постоянно хранить в МОЗУ как саму программу, так и необходимый объем проверяемой информации. Таким способом осуществляется проверка в варианте программы СИЕСК [3] для машины IBM 7030. Для хранения обрабатываемой информации здесь резервируется 70 тысяч ячеек памяти в МОЗУ.

Однако в тех случаях, когда оперативная память машины не столь велика, организация процесса проверки данных в библиотеке представляет известные трудности. Здесь приходится использовать при работе магнитные барабаны, ленты или другие носители и применять их для хранения как проверяемой информации, так и самих программ проверки. Все это, естест-

венно, усложняет работу и заставляет существенным образом учитывать при создании программы возможности и ресурсы конкретных машин.

Описываемый здесь вариант программы проверки написан на языке АЛГОЛ-60 и транслирован для машины М-220 транслятором ТА-2 [4], который эксплуатируется в ФЭИ и использует при своей работе соответствующее математическое обеспечение, отчасти также созданное в ФЭИ. Все это, конечно, наложило определенный отпечаток на программу и на те алгоритмы проверки, которые легли в ее основу.

В программе принят такой алгоритм проверки, при котором в оперативной памяти машины в каждый данный момент находится сравнительно небольшой стандартного размера массив проверяемых данных. Карты в массиве проверяются последовательно одна за другой. Это дает возможность без специального предварительного распределения оперативной памяти производить проверку массивов, имеющих переменную длину, даже в тех случаях, когда они не помещаются в ЮЗУ целиком.

В процессе работы программа ПОСОШОК проверяет:

1) правильность нумерации перфокарт в секции и секций в файле;

2) соответствие информации, включенной в нулевую секцию, заголовкам и фактическому содержанию последующих секций файла;

3) согласованность между различного рода заголовками и фактическим содержанием массивов данных внутри секции, которым эти заголовки предпосланы;

4) допустимость значений для тех или других величин, исходя из их физической природы или способа определения;

5) упорядоченность данных в пределах некоторого массива;

6) непротиворечивость друг другу различных величин, если они связаны между собой определенной зависимостью;

7) правильность нормировки угловых распределений и энергетических спектров вторичных нейтронов;

8) плавность хода нейтронных сечений и специальных величин, заданных в виде детальной энергетической зависимости (проверка на "выбросы").

Программа ПОСОШОК обрабатывает информацию, представленную в формате библиотеки рекомендованных ядерных данных, который предложен в работе [2]. Описываемый здесь вариант программы имеет дело со следующими классами ядерно-физических данных:

а) нейтронные сечения (НОК = 01),
б) угловые распределения вторичных частиц (НОК = 02),
в) энергетические распределения вторичных частиц (НОК = 03),
г) специальные величины для нейтронов (НОК = 05).

Для указанных НОК программа охватывает все основные НТП, рекомендованные в работе [2] и используемые в настоящее время на практике.

В программе пока не предусмотрена проверка данных по энерго-угловым распределениям рассеяния тепловых нейтронов (НОК = 04), формат хранения которых описан в [2]. Это связано с тем обстоятельством, что в нашем

распоряжении не было таких данных. Другие значения НОК в [2] не определены. В частности, не определены НОК, относящиеся к данным по взаимодействию фотонов с веществом. Рекомендованные ядерные данные такого рода также отсутствуют.

С появлением новых НОК или отдельных новых НТП для уже известных НОК программа должна быть расширена. В частности, все большую роль в будущем будут играть всевозможные параметрические представления данных, например, представления данных с помощью резонансных формул в области разрешенных резонансов или с помощью статистических данных для случая неразрешенных резонансов.

Структура программы ПОСОШОК легко позволяет производить такое расширение. Кроме того, имеется возможность использовать уже готовые блоки программы проверки нейтронных данных для проверки данных по взаимодействию фотонов и фотонным продуктам, если разумно подойти к выбору соответствующих форматов представления, приняв их, например, подобными форматам данных для нейтронных взаимодействий.

Как и любая машинная программа проверки данных, программа ПОСОШОК имеет определенные пределы применимости. Она в состоянии учявить только разного рода непоследовательности в данных и противоречия в формате. Некоторые ошибки в ядерных данных поэтому не будут обнаружены программой проверки и могут быть замечены только с помощью визуальной проверки. Так, например, программа в состоянии найти неверно записанное сечение в виде отрицательного числа, однако она не сможет указать на ошибку в величине Q, если, скажем, вместо правильного значения 3,607 ошибочно набито 3.067.

Поэтому потребители библиотечных данных всегда должны учитывать возможность появления ошибок, которые до сих пор оставались незамеченными. Неожиданные величины, полученные для групповых сечений, могут явиться следствием ошибок в библиотечных данных, использованных для усреднения групповых констант.

3. Структура программы

Программа ПОСОШОК в настоящее время включает в себя три блока, каждый из которых представляет собой автономно работающую программу, проверяющую данные с определенным НОК:

1. Блок ПНС – проверки нейтронных сечений (НОК = 01). Этот блок проверяет также информацию по специальным величинам для нейтронов (НОК = 05). Кроме того, в начале блока имеется особая подпрограмма для проверки нулевой (заголовочной) секции файла.
2. Блок ПУР – проверки угловых распределений (НОК = 02).
3. Блок ПЭР – проверки энергетических распределений (НОК = 03).

Все блоки программы ПОСОШОК записаны на отдельной программной магнитной ленте (ПМЛ). Данные, подлежащие проверке, хранятся на особой информационной магнитной ленте (ИМЛ) в посекторной записи.

Работа блоков программы проверки в нужном порядке осуществляется с помощью специальной программы управления работой блоков – ПУРБ, которая также записана на ПЗЛ. С ее помощью производится поиск требуемого блока на ПЗЛ, перепись его на магнитные барабаны и настройка на заданный режим работы, а также осуществляется подвод очередного сектора ПЗЛ с данными для проверки. Программа ПУРБ в течение всего времени работы программы ПОСОШОК постоянно находится в МОЗУ и написана в кодах машины М-20.

Для считывания проверяемых ядерно-физических данных с ПЗЛ в МОЗУ и для выборки затребованного кода используется административная система (АС) [4]. Поскольку в программе ПОСОШОК обработка информации идет последовательно карта за картой в порядке их следования, то применение АС оказывается весьма эффективным.

Каждый блок программы ПОСОШОК, в свою очередь, состоит из ряда написанных на языке АЛГОЛ и отдельно транслированных подпрограмм, работа которых в необходимой последовательности обеспечивается с помощью процедуры – кода „NEXT". В описываемом здесь варианте программы ПОСОШОК осуществлено следующее разбиение блоков на отдельные подпрограммы:

Блок ППС

ПЗС – проверка заголовочной (нулевой) секции
ОПС – общая проверка секций
ПСМ – проверка согласованности массивов
ПНТП – проверка НТП

Блок ПУР

ОПС – общая проверка секций
ПСМ и ПНТП – проверка согласованности массивов и НТП.

Блок ПЗР

ОПС – общая проверка секций
ПСМ – проверка согласованности массивов
ПНТП – проверка НТП.

Блок-схемы программы ПОСОШОК даны в приложении I. Алгольные тексты всех подпрограмм приводится в приложении II. Там же приведена кодовая программа ПУРБ.

Деление программы ПОСОШОК на блоки, а блоков на отдельные подпрограммы вызвано малым объемом оперативной памяти того класса машин, для которых эта программа предназначена. Тем не менее описанная здесь структура программы и связанное с этим трехступенчатое использование запоминающих устройств обеспечивает более или менее оптимальную обработку больших массивов информации на ЭВМ со сравнительно небольшим объемом МОЗУ. Кроме того, и это очень важно для будущего, такая структура дает возможность подсоединять к программе новые блоки и включать отдельные новые подпрограммы внутрь уже существующих блоков, если в этом возникнет потребность, без особой перестройки всей программы.

Следует также отметить, что реализованная для целей проверки структурная схема позволяет, наряду с программой ПОСОШОК, эксплуатировать также и некоторые другие программы из комплекса обслуживающих библиотеку рекомендованных ядерных данных программ. В частности, уже в настоящее время в эту систему включена программа перевода данных из формата библиотеки NDL [5] в формат, принятый в ФЭИ.

4. Ресурсы памяти машины

Предполагается, что оперативная память машины состоит из одного куба емкостью 4096 ячеек и распределяется для программы ПОСОШОК следующим образом (указаны восьмеричные адреса ячеек МОЗУ):

0000-0012 - рабочие ячейки.
0013-0143 - программа АС.
0144-6553 - подпрограмма, работающая в МОЗУ, рабочее поле АС, поля для переменных и массивов. Фактическое распределение этого объема МОЗУ производится транслятором.
6554-6777 - рабочая память программы, распределяемая программистом с помощью комментариев. Описание идентификаторов, используемых в программе переменных, дается в приложении II вместе с текстами соответствующих программ.
7000-7177 - управляющая программа ПУРБ.
7200-7777 - используются при работе ИС-2 [6].

При работе программы ПОСОШОК могут использоваться все четыре имеющихся на машине магнитных барабана емкостью по 4096 ячеек каждый[x]. Нулевой МБ отводится под ИС. Три остальных барабана служат для хранения работающего в данный момент блока программы.

Подпрограммы блока располагаются начиная с первого МБ и, если требуется, переходят на второй и третий барабаны. При этом требуется, чтобы блок программы целиком помещался на магнитных барабанах. Ячейки с адресами 7640-7777 на МБ-3 занимаются паспортом работающего блока. Такой паспорт формируется во время записи блока на ПМЛ и используется для организации поочередного вызова с МБ в МОЗУ подпрограмм данного блока с помощью процедуры-кода „NEXT".

Для своей работы программа ПОСОШОК требует две ленты: ПМЛ, куда записаны блоки самой программы, включая управляющую программу ПУРБ, и ИМЛ, где в посекторной записи хранятся файлы проверяемых данных. Информация на магнитных лентах (как на ПМЛ, так и на ИМЛ) хранится стандартными зонами по 129 кодов в каждой.

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x) Под барабаном понимается здесь четвертая часть полного (нулевого) барабана емкостью 16384 ячейки.

Программная магнитная лента размечена на стандартные зоны, нумерация которых начинается с единицы. В первую зону ПМЛ записывается управляющая программа ПУРБ. Вторую зону занимает паспорт программы (системы блоков), а в зоны начиная с третьей записываются блоки программы в порядке их следования. Всякий новый блок программы пишется с новой зоны. В конце блока могут быть оставлены пустые зоны, которые оказываются полезными в том случае, когда возникает необходимость перезаписи блока или внесения в него возможных исправлений.

Паспорт системы блоков формируется в процессе записи блоков на ПМЛ. Каждый блок в таком паспорте характеризуется кодом следующего вида:

$$0 \quad 52 \qquad 0000 \qquad \text{ЧЗБ}(i) \qquad 0000,$$

где ЧЗБ(i) восьмеричное число зон, отведенных для i -го блока программы. Паспорт позволяет определить местоположение любого блока программы на ПМЛ. При работе программы ПОСОШОК это делается с помощью управляющей программы ПУРБ.

В свою очередь каждый блок программы на ПМЛ начинается с паспорта блока, который занимает первую зону, отведенную под данный блок. Далее следуют подпрограммы этого блока, каждая из которых начинается с новой зоны.

Подлежащие проверке ядерно-физические данные хранятся на информационной магнитной ленте и представлены в формате Библиотеки рекомендованных ядерных данных ФЭИ [2]. Предполагается, что ИМЛ разбита на сектора, каждый из которых, в свою очередь, размечен на стандартные зоны с автономной нумерацией. Посекторная запись дает возможность обращаться с секторами как с независимыми магнитными лентами. Кроме того введение секторов позволяет существенно увеличить суммарное количество зон на магнитной ленте, не ограничивая при этом работу АС, которая, как известно [4], требует, чтобы число стандартных зон на МЛ не превышало определенного значения.

Каждый файл данных занимает отдельный сектор ленты. В первый сектор записывается заголовок длиной ИМЛ. Заголовок содержит сведения о количестве файлов на ленте и, возможно, некоторую другую информацию о каждом из них. Ввод ядерных данных с перфокарт в МОЗУ и запись их на ИМЛ производится с помощью специальной программы.

5. Начальная информация

Для работы программы ПОСОШОК должна быть заготовлена некоторая начальная информация, которая набивается на перфокартах и располагается при вводе в следующем порядке:

1. Стандартная карта вызова ИС-2.
2. Карта вызова ПУРБ с ПМЛ.

3. Исходная информация для работы:

а) 0 00 ЧФ 0000 0000

б) ПВПД

Далее для каждого i -го ($1 \leq i \leq ЧФ$) проверяемого файла с данными задается:

в) 0 00 НС (i) 0000 0000

Для каждого следующего файла, подлежащего проверке, данные пункта "в" повторяются

4. Контрольная сумма исходной информации для работы.

Здесь ЧФ – количество подлежащих проверке файлов,

НС(i) – информация для подвода сектора, в котором находится i -й по порядку файл проверяемых данных (из общего числа ЧФ файлов),

ПВПД – признак вида проверки данных.

Значения ЧФ и НС представляют собой восьмеричные числа, пробитые по первому адресу. Первый разряд числа НС отводится под программный номер магнитофона, а три остальных младших разряда определяют порядковый номер сектора на магнитной ленте. Десятичная константа ПВПД имеет следующие значения:

ПВПД = 0 – полная проверка,
= 1 – только общая проверка.

Карта вызова ПУРБ с ПМЛ имеет вид:

0	I6	0000	0020	0000
0	00	0020	0000	0000 КА
0	I6	002I	7500	76I0
0	23	7000	000I	7I76
0	I6	НБ	700I	7000
0	75	7042 + НБ	6524	6006 КС

Здесь НБ – восьмеричный номер блока, который должен быть вызван для работы первым.

6. Работа программы в процессе проверки

Проверка данных любого файла проводится по секциям в порядке их следования. Для каждой секции проверка происходит в два этапа:

первый этап – общая проверка,
второй этап – детальная проверка.

На первом этапе работает подпрограмма общей проверки секции; при этом выявляются лишь те ошибки, которые не связаны с определенным типом реакции. Такие ошибки будут называться общими ошибками. На втором этапе в работу включаются другие подпрограммы, которые осуществляют детальную проверку данной секции.

Для любой секции сначала производится общая проверка. Затем, если ПКПД в исходных данных требует полной проверки и если при общей проверке секции не встретилось ошибок, которые могут привести к нецелесообразности дальнейшей проверки составных частей этой секции, происходит переход к детальной проверке данной секции. В противном случае происходит переход к проверке следующей секции.

Проведение проверки в два этапа целесообразно по следующим соображениям. Поскольку поиск всех ошибок идет параллельно по картам, то может оказаться, что многие ошибки общего характера, влияющие на ход последующей проверки и делающие такую проверку нецелесообразной, будут обнаружены в самом конце проверки. В этом случае будет проделана заведомо бесполезная работа и выдана обширная информация о фиктивных ошибках, которая не может быть использована для выявления истинных ошибок.

Процесс проверки данных по программе ПОСОШОК полностью автоматизирован, сопровождается периодической выдачей результатов проверки на печеть и идет без вмешательства оператора. Опишем в общих чертах последовательность работы программы ПОСОШОК в процессе проверки данных (см. приложение I).

Вызванная с ПМЛ в МОЗУ управляющая программа ПУРБ осуществляет ввод необходимой для работы исходной информации, по имеющемуся в ней номеру НС(I) подводит сектор ИМЛ с первым по порядку файлом проверяемых данных, а затем вызывает с ПМЛ на магнитные барабаны блок программы, номер которого указан в карте вызова ПУРБ. При работе в режиме проверки это будет первый блок программы ПОСОШОК – блок ПНС, который записан в начале ПМЛ.

Если однако по каким-либо причинам в начале работы программой ПУРБ требуется вызвать на МБ не первый по порядку блок, записанный на ПМЛ, а блок с более высоким номером, то именно этот номер и следует указать в "Карте вызова ПУРБ с ПМЛ". Так, например, при работе в режиме перевода первым должен вызываться начальный блок программы перевода. Для программы перевода данных из формата *NDL* [5] в формат ФЭИ такой блок записан на ПМЛ четвертым, вслед за тремя блоками программы ПОСОШОК. В данном случае в карте вызова ПУРБ указывается номер этого блока.

Вызов соответствующего блока с ПМЛ производится следующим образом. Сначала с ленты в МОЗУ считывается паспорт системы блоков и по заданному номеру блока отыскивается начало нужного блока на ПМЛ. Затем в МОЗУ списывается паспорт блока, с его помощью переписываются на магнитные барабаны все подпрограммы данного блока, а также сам паспорт блока, и по коду " *NEXT* " с МБ в МОЗУ для работы вызывается первая по порядку подпрограмма блока.

Программа ПОСОШОК всегда начинает свою работу с вызова в МОЗУ и работы подпрограммы ПЗС первого блока программы (блока ПНС), поскольку предполагается, что в любом проверяемом файле должна иметься заголовочная (нулевая) секция, расположенная в начале файла. При повторных обращениях к этому блоку в пределах данного файла подпрограмма ПЗС вызывается, но не работает и управление из нее передается на вызов с МБ следующей подпрограммы данного блока - подпрограммы ОПС.

По окончании проверки нулевой секции происходит настройка программы на проверку следующей секции. Такая настройка включает в себя выделение и анализ НОК подлежащей проверке секции. Если при этом окажется, что в программе имеется соответствующий блок для проверки данных с таким НОК, но этот блок не находится в данный момент на МБ, то происходит вызов этого блока с ПМЛ. Во всех остальных случаях для проверки очередной секции используется блок, находящийся на МБ. Вызов нового блока с ПМЛ на МБ осуществляется через посредство управляющей программы ПУРБ.

При вызове любого нового блока работа его начинается с первой по порядку подпрограммы. Напротив, в том случае, когда для проверки первой секции остается блок, уже находящейся на МБ, к работе приступает следующая подпрограмма этого блока. Таким образом, после проверки заголовка файла и выполнения соответствующей настройки программы на проверку следующей секции, в работу всегда включается подпрограмма ОПС того или иного блока программы ПОСОШОК. Начинается первый этап проверки - общая проверка данной секции.

Если для файла требуется лишь общая проверка (ПВПД = I), переход к проверке следующей секции происходит непосредственно внутри данной подпрограммы ОПС. В результате общая проверка всех секций данного файла будет произведена одной подпрограммой, постоянно находящейся в МОЗУ, без обращения к МБ или МЛ, что позволяет существенно сократить общее время работы программы.

Напротив, когда для файла необходима полная проверка (ПВПД = 0), но в секции при общей проверке встретились ошибки, влияющие на ход дальнейшей проверки, осуществляется предварительная настройка программы на проверку следующей секции, как это было описано выше. Если при этом окажется, что соответствующий этой секции блок проверки уже находится на МБ, то общая проверка такой секции также будет производиться подпрограммой ОПС, в данный момент находящейся в МОЗУ.

Наконец, в том случае, когда признак ПВПД требует для файла полной проверки и при работе подпрограммы ОПС в секции не было обнаружено ошибок, влияющих на проверку, то с помощью " NEXT " вызывается в МОЗУ и приступает к работе следующая по порядку подпрограмма данного блока - подпрограмма ПСМ.

Подпрограммы ПСМ и ПНТП любого блока осуществляют второй этап проверки - детальную проверку секции. В процессе этой проверки они поочередно вызываются в МОЗУ с МБ и выполняют свои функции до тех пор, пока не будут полностью исчерпаны все имеющиеся НТП при всех температурах (группах вторичных частиц) и для всех энергетических интервалов данной секции. При этом каждое обращение к подпрограмме ПНТП и проверка ошибок для соответствующего НТП происходит только в том случае, когда с помощью

подпрограммы ПСМ предварительно проверена согласованность всех массивов, внутри которых расположен данный массив НТП, включая также проверку согласованности и самого массива НТП, и при такой проверке не встретилось ошибок, ведущих к прекращению дальнейшей проверки какого-либо из этих массивов. Если проверенная таким образом секция не была последней в файле, производится настройка программы на проверку следующей секции и осуществляется переход к подпрограмме ОПС соответствующего блока.

По окончании проверки последней секции данного файла происходит обращение к управляющей программе ПУРБ для подвода очередного сектора с новым файлом проверяемых данных и, если это необходимо, для вызова с ПМЛ на МБ требуемого блока программы. Работа программы ПОСОШОК заканчивается после того, как будут проверены все файлы, для которых в исходной информации заданы номера содержащих их секторов.

7. Классификация ошибок

Любая ошибка в библиотечных рекомендованных данных, которая анализируется с помощью программы ПОСОШОК, характеризуется своим специальным кодовым числом – Номером Типа Ошибки (НТО). В таком закодированном виде под соответствующими НТО ошибки выдаются на печать в качестве результатов проверки.

Все проверяемые программой ПОСОШОК ошибки разбиваются на две категории.

1. Ошибки, не влияющие на ход проверки и
2. Ошибки, которые делают нецелесообразной последующую проверку какого-либо массива данных.

Два однотипных массива информации, например две секции или два массива с данными для определенных энергетических интервалов, будем называть массивами одного и того же ранга. Напротив, если какой-либо массив полностью включает в себя один или несколько других массивов, имеем дело с массивами разных рангов. При этом охватывающий массив будет иметь более высокий, а вложенные массивы более низкие ранги. Ранги массивов могут отличаться на одну или несколько единиц. Так, например, ранги файла и содержащейся в нем секции отличаются на единицу, а ранги файла и входящего в эту секцию некоторого энергетического интервала отличаются на 2 единицы.

Среди ошибок, влияющих на дальнейшую проверку, можно выделить следующие классы ошибок.

А. Ошибки, появление которых требует прекращения только общей проверки данной секции с дальнейшим переходом на проверку следующей секции.

Б. Ошибки, требующие проверки только минимально допустимого числа (одного-двух) очередных массивов, после чего осуществляющие переход к проверке следующего массива более высокого ранга.

В. Ошибки, прекращающие проверку данного массива и требующие перехода к проверке следующего массива того же или более высокого ранга.

НТО указанных классов ошибок будут в дальнейшем приводиться вместе с соответствующими буквами, под которыми они стоят в данном перечислении.

Целый ряд НТО касаются структуры отдельных массивов и устанавливают соответствие между их содержанием и заголовками. Определим некоторые формулировки, относящиеся к такого рода ошибкам. Будем говорить, что:

а) массив несовместен, если число входящих в него подмассивов не равно значению этой величины, приведенному в заголовке массива,

б) массив противоречив, если число карт, содержащихся в данном массиве, не равно значению этой величины, приведенному в заголовке массива,

в) массив не согласован, если число карт, содержащихся в данном массиве, не равно значению этой величины, определенному для массива заголовками всех входящих в него подмассивов, число которых указано в заголовке массива.

Ниже дается описание НТО, используемых для кодирования ошибок, проверяемых программой ПОСОШОК. Данные представлены в виде таблицы, в которой приводятся значения НТО и их расшифровка.

Таблица

Описание ошибок,
проверяемых программой ПОСОБОК

I) Ошибки, не связанные с определенным типом реакции.
(Общие ошибки)

НТО	Расшифровка
I0 A	Значение НТО в заголовке секции не равно НТР, определенному для этой секции заголовком файла (нулевой секцией).
II A	НОК в заголовке секции недопустим ($0 \geqslant$ НОК $\geqslant 6$ или НОК = 4).
I2	НЧК в заголовке секции не допустим ($0 \geqslant$ НЧК $> I08$)
I3 на карте n	Величина $bH?xIC^4 + nC$ в поле меток карты n не равна значению этой же величины на первой карте секции.
I4 на карте n	Величина $bH?xIC^4 + nC$ в поле меток карты n не равна значению этой же величины на предыдущей карте секции.
I5 на карте n (упоминается номер N)	Номер карты (N), указанный в поле меток, не равен порядковому номеру n этой карты в секции. (Порядковый номер на карте не верен).
I6 на карте n (упоминается номер N)	Номер карты (N), указанный в поле меток, не равен увеличенному на единицу значению этой же величины на предыдущей ($n-1$) карте секции. (Не монотонный рост номеров карт в секции).
I7	Число карт в секции не равно числу карт, указанному для этой секции в заголовке файла. (Секция противоречива).
I8A	Число карт в секции не равно числу карт, определенному для этой секции заголовками всех входящих в нее энергетических интервалов. (Секция не согласована).
I9	Число энергетических интервалов (ΔE), входящих в секцию, не равно числу ΔE , указанному в заголовке секции. (Секция не совместна).
20	Число карт в файле не равно полному числу карт для файла, указанному в его заголовке. (Файл противоречив).

НТО	Расшифровка
2I	Число секций в файле не равно числу НТР, указанному на первой карте заголовка файла. (Файл не совместен).

2) Ошибки в заголовке файла (в нулевой секции)

НТО	Расшифровка
50	Атомный номер Z, заданный на первой карте, отрицателен ($Z < 0$).
5I	Атомный (молекулярный) вес A, заданный на первой карте, отрицателен или равен нулю ($A \leq 0$).
52	Число НТР и число карт в нулевой секции, заданные на первой карте, не совместимы.
53 секция l (упоминается номер L)	Номер секции (L), указанный в заголовке файла, не равен порядковому номеру l следования этой секции в том же заголовке. (Порядковый номер секции в заголовке файла не верен).
54	Число карт в нулевой секции не равно числу карт, указанному для этой секции на первой карте. (Нулевая секция противоречива).
55	Полное число карт файла, указанное в заголовке, не равно сумме приведенных в том же заголовке чисел карт для всех входящих в этот файл секций. (Файл не согласован).
56	Число НТР для вещества, указанное на первой карте заголовка файла, не совпадает с количеством НТР, перечисленных в нулевой секции.

3) Ошибки в данных по нейтронным сечениям (НОК=0I) и специальным величинам для нейтронов (НОК = 05)

НТО	Расшифровка
I0I	Значение Q для полного сечения или сечения упругого рассеяния, заданное на первой карте секции, отлично от нуля.

НТО	Расшифровка
I02	Вычисленная для данной реакции пороговая энергия превышает нижнюю границу первого ΔE .
I03 на карте n	Нижняя граница ΔE , заданная на карте n , меньше верхней границы предыдущего ΔE (перекрывание энергетических интервалов).
I04Б на карте n	Число температур для ΔE , указанное на карте n , меньше I.
I05В на карте n	Массив ΔE (заголовочная карта n) не согласован.
I06 на карте n (упоминается карта m)	Температура T на карте n отлична от нуля, хотя число температур, указанное в заголовке ΔE (карта m), не предполагает существование температурной зависимости (число T равно I).
I07 на карте n (упоминается карта m)	Температура T на карте n равна нулю, хотя число температур, указанное в заголовке ΔE (карта m), предполагает существование температурной зависимости (число T меньше I).
I08 на карте n	Температура T, заданная на карте n , отрицательна.
I09Б на карте n	Число НТП для температуры T , указанное на карте n , меньше I.
IIOВ на карте n	Массив температуры T (заголовочная карта n) не согласован.
IIIВ на карте n	НТП на заголовочной карте n не допустим.
II2Б на карте n	Для НТП = I0I число значений НТП, указанное в заголовке для T (карта n), больше I.
II3 на карте n	Число карт для НТП = I0I, указанное на карте n , не равно I.
II4 на карте n	Нижняя граница ΔE , заданная для НТП = I0I на карте n , не положительна.

НТО	Расшифровка
II5 на карте n	Нижняя граница ΔE, заданная для НТП = I0I на карте n, больше (или равна) его верхней границы.
II6B на карте n	Число карт и число значений E, приведенных для НТП = III в заголовке (карта n), не совместны.
II7B на карте n	Число значений E для данного НТП, указанное на карте n, меньше 2 (для НТП = III) или меньше I (для НТП = I2I).
II8B на карте n	Массив НТП = I2I (заголовочная карта n) не согласован.
II9 на карте n (упоминается карта m)	Первое значение E для данного НТП (карта n) не совпадает с нижней границей ΔE, заданной на карте m.
I20 в точке S (карта n)	Энергия E в точке S (на карте n) не положительна.
I2I в точке S (карта n)	Значение E в точке S (на карте n) не входит в монотонно возрастающую последовательность значений энергий для данного НТП.
I22 в точке S (карта n)	Сечение σ в точке S (на карте n) не положительно.
I23 в точке S (карта n)	Значение σ в точке S (на карте n) выпадает из плавного хода энергетической зависимости сечений для данного НТП ("выброс", это значение σ подозревается на ошибку).
I24 на карте n (упоминается карта m)	Последнее значение E для данного НТП (карта n) не совпадает с верхней границей ΔE, заданной на карте m.
I25B на карте n (упоминается карта m)	Число подгрупп при энергии E, заданное на карте n, не равно числу подгрупп, указанному в заголовке НТП (карта m), если число подгрупп не зависит от E.
I26B на карте n	Число подгрупп для данного E, указанное на карте n, меньше I.

НТО	Расшифровка
I27 в подгруппе i (карте n)	Доля a_i для подгруппы i (на карте n) не положительна.
I28 в подгруппе i (карте n)	Сечение σ_i для подгруппы i (на карте n) не положительно.
I29 в подгруппе i (карте n)	Значение σ_i для подгруппы i (на карте n) не входит в монотонно возрастающую (упорядочению) последовательность подгрупповых сечений при данном E.
I30	Сумма a_i по всем подгруппам для данного E отличается от I на величину большую, чем $0{,}5N \cdot 10^{-6}$, где N -число подгрупп.

4) Ошибки в данных по угловым распределениям нейтронов (НОК = 02)

НТО	Расшифровка
200	Значения величин A в заголовке данной секции и в заголовке файла не равны друг другу.
201 на карте n	Нижняя граница первого Δ E, заданная на карте n, не положительна.
202 на карте n	Нижняя граница Δ E, заданная на карте n, больше (или равна) его верхней границы.
203 на карте n	Нижняя граница ΔE, заданная на карте n, меньше верхней границы предыдущего ΔE (перекрывание энергетических интервалов).
204 на карте n	Значения границ ΔE, заданные на карте n, указывают на возможность того, что данный ΔE не входит в упорядоченную последовательность ΔE для секции (возможное перепутывание энергетических интервалов).
205Б на карте n	Число групп вторичных частиц для ΔE, указанное на карте n, меньше I.

206В на карте n — Число проверенных (включая данную) групп вторичных частиц для ΔE меньше того значения, которое указано в заголовке этого ΔE (карта n), но число карт, определенное заголовками проверенных в данном ΔE групп, больше (или равно) числа карт для ΔE, указанного в его заголовке.

207В на карте n — Число карт для ΔE, указанное в его заголовке (карта n), не равно числу карт, определенному для этого ΔE заголовками всех имеющихся в нем групп вторичных частиц, число которых также указано в заголовке данного ΔE.

208 на карте n — Условное число группы вторичных частиц, заданное на карте n, не входит в упорядоченную последовательность значений этого числа для данного ΔE.

209 — Сумма условных чисел, отождествляющих группы вторичных частиц для ΔE, не согласуется с числом вторичных частиц в данной реакции, определяемым НТР.

210Б на карте n — Число НТП для группы частиц, указанное на карте n, меньше I.

211В на карте n — НТП на заголовочной карте n не допустим.

212В на карте n — Число проверенных (включая данный) НТП для группы вторичных частиц меньше того значения, которое указано в заголовке этой группы (карта n), но число карт, определенное заголовками проверенных в группе НТП, больше (или равно) числа карт для этой группы, указанного в ее заголовке.

213В на карте n — Число карт для группы вторичных частиц, указанное в ее заголовке (карта n), не равно числу карт, определенному для этой группы заголовками всех относящихся к ней НТП, число которых также указано в заголовке данной группы частиц.

НТО	Расшифровка
214 на карте n	Условное число системы отсчета, заданное для НТП на карте n, не допустимо.
215 на карте n	Для НТП = 101 или НТП = 201 указанное в заголовке группы вторичных частиц (карта n) число НТП больше 1.
216Б на карте n	Число значений Е для данного НТП, указанное в его заголовке на карте n, меньше 2.
217В на карте n	Число проверенных (включая данное) значений Е для НТП меньше того значения, которое указано в заголовке этого НТП (карта n), но число карт, определенное заголовками проверенных в данном НТП значений Е, больше (или равно) числа карт для НТП, указанного в его заголовке.
218В на карте n	Число карт для НТП, указанное в его заголовке (карта n), не равно числу карт, определенному для этого НТП заголовками всех входящих в него значений E, число которых также указано в заголовке данного НТП.
219 на карте n (упоминается карта m)	Первое значение Е для данного НТП (карта n) не совпадает с нижней границей ΔE, заданной на карте m.
220 на карте n	Энергия Е для НТП, заданная на карте n, не положительна.
221 на карте n	Значение Е на карте n не входит в монотонно возрастающую последовательность значений энергий, заданных для данного НТП.
222 на карте n (упоминается карта m)	Последнее значение Е для данного НТП (карта n) не совпадает с верхней границей ΔE, заданной на карте m.
223Б на карте n	Число значений α для данного Е (или НТП), указанное в соответствующем заголовке на карте n, меньше 1 для Е (или меньше 2 для НТП).
224В на карте n	Число проверенных (включая данное) значений α или Е (или для НТП) меньше того значения, которое указано в соответствующем заголовке Е (или НТП) на карте n,

КТО	Расшифровка
	но число карт, определенное заголовками проверенных для данного E (НТП) значений a, больше (или равно) числа карт для этого E (НТП), указанного в его заголовке.
225B на карте n	Число карт для E (или для НТП), указанное в соответствующем заголовке (карта n), не равно числу карт, определенному для этого E (или НТП) заголовками всех относящихся к нему значений a, число которых указано в заголовке E (НТП).
226 на карте n	Доля распределения a, относящегося к данному E (или НТП), заданная на заголовочной карте n, не положительна.
227E на карте n	Число значений μ (или ω), указанное на соответствующей карте n, меньше 2.
228 на карте n	Первое значение μ (карта n) не равно – I.
229 в точке S (карта n)	Значение μ в точке S (на карте n) не входит в монотонно возрастающую последовательность значений μ.
230 в точке S (карта n)	Значение $f(\mu)$ в точке S (на карте n) не положительно.
231 на карте n	Последнее значение μ (карта n) не равно + I.
232	Сумма a по всем частичным распределениям в данном компоненте для данного E (или НТП) отличается от I на величину большую, чем $0{,}5N\cdot10^{-6}$, где N – число распределений в компоненте.

5) Ошибки в данных по энергетическим распределениям вторичных нейтронов (НОК = 05)

НТО	Расшифровка
301 на карте n	Нижняя граница первого ΔE, заданная на карте n, не положительна.
302 на карте n	Нижняя граница ΔE, заданная на карте n, больше (или равна) его верхней границы.
303 на карте n	Нижняя граница ΔE, заданная на карте n, меньше верхней границы предыдущего ΔE (перекрытие энергетических интервалов).
304 на карте n	Значения границ ΔE, заданные на карте n, указывают на возможность того, что данный ΔE не входит в упорядоченную последовательность ΔE для секции (возможное перепутывание энергетических интервалов).
305Б на карте n	Число групп вторичных частиц для ΔE, указанное на карте n, меньше I.
306В на карте n	Число проверенных (включая данную) групп вторичных частиц для ΔE меньше того значения, которое указано в заголовке ΔE (карта n), но число карт, определенное заголовками проверенных в ΔE групп, больше(или равно) числа карт для этого ΔE, указанного в его заголовке.
307В на карте n	Число карт для ΔE, указанное в его заголовке (карта n), не равно числу карт, определенному для этого ΔE заголовками всех входящих в него групп вторичных частиц, число которых также указано в заголовке ΔE.
308 на карте n	Условное число группы вторичных частиц, заданное на карте n, не входит в упорядоченную последовательность значений этого числа для данного ΔE.
309	Сумма условных чисел, отождествляющих группы вторичных частиц для ΔE, не согласуется с числом вторичных частиц в данной реакции, определяемым НТР.

НТО	Расшифровка
3I0 на карте n	Число НТП для группы частиц, указанное на карте n, меньше I.
3I1B на карте n	НТП на заголовочной карте n не допустим.
3I2B на карте n	Число проверенных (включая данный) НТП для группы вторичных частиц меньше того значения, которое указано в заголовке этой группы (карта n), но число карт, определенное заголовками проверенных в группе НТП, больше (или равно) числа карт для этой группы, указанного в ее заголовке.
3I3B на карте n	Число карт для группы вторичных частиц, указанное в ее заголовке (карта n), не равно числу карт, определенному для этой группы заголовками всех относящихся к ней НТП, число которых также указано в заголовке данной группы частиц.
3I4B на карте n	Число значений E_0 для данного НТП, указанное в его заголовке на карте n, меньше 2.
3I5B на карте n	Число проверенных (включая данное) значений E_0 для НТП меньше того значения, которое указано в заголовке этого НТП (карта n), но число карт, определенное заголовками проверенных в данном НТП значений E_0, больше (или равно) числа карт для этого НТП, указанного в его заголовке.
3I6B на карте n	Число карт для НТП, указанное в его заголовке (карта n), не равно числу карт, определенному для этого НТП заголовками всех входящих в него значений E_0, число которых также указано в заголовке данного НТП.
3I7 на карте n (упоминается карта m)	Первое значение E_0 для данного НТП (карта n) не совпадает с нижней границей ΔE, заданной на карте m.
3I8 на карте n	Энергия E_0 для НТП, заданная на карте n, не положительна.

НТО	Расшифровка
319 на карте n	Значение E_0 для НТП, заданное на карте n, не входит в монотонно возрастающую последовательность значений энергии для данного НТП.
320 на карте n (упоминается карта m)	Последнее значение E_0 для данного НТП (карта n) не совпадает с верхней границей ΔE, заданной на карте m.
321Е на карте n	Число различных законов в линейной комбинации для данного E_0 (или НТП), указанное в соответствующем заголовке на карте r, меньше I (или меньше 2).
322В на карте n	Номер закона для данного E_0 (или НТП) в соответствующем заголовке (карта n) не допустим.
323В на карте n	Число проверенных (включая данный) законов для E_0 (или для НТП) меньше того значения, которое указано в соответствующем заголовке E_0 (или НТП) на карте n, т.е. число карт, определенное заголовками проверенных для данного E_0 (НТП) законов, больше (или равно) числа карт для этого E_0 (НТП), указанного в его заголовке.
324В на карте n	Число карт для E_0 (или для НТП), указанное в соответствующем заголовке (карта n), не равно числу карт, определенному для этого E_0 (или НТП) заголовками всех относящихся к нему законов, число которых указано в заголовке E_0 (НТП).
325 на карте n	Номер данного закона для E_0 (НТП) на заголовочной карте n не находится в упорядоченной последовательности номеров законов, входящих в линейную комбинацию для этого E_0 (НТП).
326 на карте n	Вероятность закона в линейной комбинации для E_0 (или НТП), заданная на карте n, не положительна.
327Б на карте n	Число значений аргумента (дискретных энергий, точек спектра и т.д.), указанное в соответствующем заголовке (карта n), меньше I.

НТО	Расшифровка
328 в точке S (карта n)	Значение аргумента в точке S (на карте n) не положительно.
329 в точке S (карта n)	Значение аргумента в точке S (на карте n) не входит в монотонно возрастающую (упорядоченную) последовательность значений этого аргумента.
330 в точке S (карта n)	Для закона 2 величина k в точке S (на карте n) не удовлетворяет условию $0 < K \leq I$.
331 в точке S (карта n)	Значение вероятности p в точке S (на карте n) не положительно.
332 ...	Сумма p, соответствующих всем значениям аргумента для законов I или 2, отличается от I на величину, большую, чем $0{,}5\ N \cdot 10^{-6}$, где N - число значений аргумента.
333 на карте n	Для законов 3 или 4 значения величин A и C или a, c и E_x, заданные на карте n, не положительны.
334	Сумма вероятностей законов, входящих в линейную комбинацию для данных НТП или E_0, отличается от I на величину большую, чем $0{,}5N \cdot 10^{-6}$, где N -число законов в комбинации.

8. Выдача результатов

Результаты работы программы ПОСОШСК выдаются на широкую печать. Вывод представляет собой список НТО, обнаруженных при проверке ошибок. Во всех случаях, когда это необходимо, определяется местоположение ошибки в массиве проверяемых данных. Указывается номер карты или номера точки и карты, где обнаружена ошибка. В ряде случаев дается дополнительная ссылка на номер карты или номер значения величины, о которых имеется упоминание в расшифровке НТО. В отдельных случаях, когда это целесообразно, в печатной выдаче приводится также само значение ошибочной величины.

Ошибки группируются по массивам проверяемых данных и снабжаются соответствующими заголовками. Каждый такой заголовок определяет тот массив информации, внутри которого эти ошибки обнаружены.

Наряду с ошибками печатаются суммы вероятностей и интегралы нормированных угловых и энергетических распределений. К такого рода данным необходимо относиться с осторожностью, поскольку обнаруженные при проверках

нормализации расхождения не всегда указывают на наличие ошибок. Поэтому выданные на печать значения нормировок должны быть тщательно проанализированы, прежде чем на их основе будут сделаны заключения о наличии или отсутствии таких ошибок.

Пример печатной выдачи результатов проверки некоторого файла дается в приложении Ш. Там же приводится распечатка этого файла с имеющимися в нем ошибками.

9. Вспомогательные программы

К ним относятся программы, осуществляющие предварительную запись на магнитные ленты программы ПОСОШОК и ядерно-физических данных, подлежащих проверке. Тексты соответствующих программ даются в приложении П.

9.1. Программа записи блоков на ленту (ЗБЛ)

Организация работы по нахождению случайных ошибок в библиотечных данных предполагает, что программа ПОСОШОК уже записана на ПМЛ. Для предварительной записи ее на ленту служит специальная программа ЗБЛ - "Запись Блоков на Ленту". Программа ЗБЛ написана в кодах машины М-220 и при работе располагается в МОЗУ, начиная с адреса 5747, занимая 256 адресных кодов.

Для работы программа ЗБЛ вводится в МОЗУ с карт. Массив перфокарт формируется следующим образом:

1. Стандартная карта вызова МС-2.
2. Карта ввода программы ЗБЛ.
3. Колоде перфокарт программы ЗБЛ.
4. Исходная информация для работы.

а) ПРРБ - признак режима работы программы ЗБЛ (восьмеричный код).
ПРРБ = 0 00 0000 0000 0000 - режим первоначальной записи системы блоков на ПМЛ.
ПРРБ = 0 00 0000 0000 0001 - режим дописывания блоков на ПМЛ.
ПРРБ = 0 00 0000 0001 0000 - режим перезаписи отдельных блоков на ПМЛ.

В режиме перезаписи для каждого блока, который должен быть перезаписан, задается:

б) информация для перезаписи очередного блока на ПМЛ

0 00 НБ 0000 0000,

где НБ - восьмеричный порядковый номер перезаписываемого блока.

Для каждого следующего блока, подлежащего перезаписи, данные пункта "б" повторяются. При других режимах работы данные пункта "б" отсутствуют.

5. Контрольная сумма исходной информации для работы.
6. Колода перфокарт программы ПУРБ (только в режиме первоначальной записи).

Далее, для каждого вновь записываемого или перезаписываемого блока задается:

7. Колода перфокарт с программами данного блока.
8. Признак конца блока

7 77 7777 7777 7777
7 77 7777 7777 7777 КС.

Для каждого следующего блока, подлежащего записи или перезаписи, подкладываются данные, указанные в пунктах 7 и 8.

Блоки в массиве с данными располагаются в той последовательности, в какой они должны быть записаны на ПМЛ.

В режиме первоначальной записи в первую зону ПМЛ записывается управляющая программа ПУРБ, а в зоны, начиная с третьей, записываются блоки программы ПОСОШОК в том порядке, в каком они следуют в массиве данных для программы ЗБЛ. Параллельно с этим формируется паспорт системы блоков (паспорт программы), который затем помещается во вторую зону ПМЛ.

В режиме дописывания программа ЗБЛ по паспорту системы блоков находит последнюю занятую блоками программы зону ПМЛ и в последующие свободные зоны производит запись дополнительных блоков в порядке их следования в массиве данных для работы программы ЗБЛ. При этом происходит также внесение дополнений в паспорт программы, хранящийся во второй зоне ПМЛ.

При работе в режиме перезаписи с помощью паспорта программы находятся на ПМЛ те блоки, номера которых указаны в исходной информации для работы программы ЗБЛ, и на их место записываются вводимые с перфокарт блоки в том порядке, в каком они следуют в массиве задаваемой информации. При этом необходимо следить за тем, чтобы объем вводимого с перфокарт блока не выходил за пределы того объема НЗУ, который был отведен под ранее записанный блок программы. Важное значение могут здесь иметь свободные резервные зоны, оставленные при первоначальной записи блоков.

В программе ЗБЛ реализован следующий порядок работы. После ввода с перфокарт и записи (или перезаписи) на ленту очередного блока программа выходит на "Останов". Ввод следующего блока осуществляется нажатием кнопки "Пуск" на пульте управления. В случае сбоя при вводе колода карт вместе с признаком конца блока ставится в читающее устройство еще раз и производится повторное нажатие кнопки "Пуск".

9.2. Программа записи данных на ленту (ЗДЛ)

При работе программы ПОСОШОК предполагается, что подлежащие проверке ядерно-физические данные находятся на ПМЛ. Поскольку ввод с перфокарт и

запись на ленту больших массивов информации сама по себе есть работа трудоемкая и кропотливая, то эту работу целесообразно провести заранее с помощью специальной программы ЗДЛ - "Запись Данных на Ленту".

Программа ЗДЛ написана в кодах ..ВК и занимает при работе в МОЗУ 140 адресных кодов, начиная с адреса 6775. Запись информации происходит в предварительно размеченные с помощью особой программы разметки сектора НМЛ.

Массив перфокарт для работы программы ЗДЛ составляется следующим образом.

1. Стандартная карта вызова МС-2.
2. Карта ввода программы ЗДЛ.
3. Колода перфокарт программы ЗДЛ.
4. Исходная информация для работы:

а) информация о количестве записываемых файлов с данными

0 00 ЧФ 0000 0000,

где ЧФ - число подлежащих записи файлов (восьмеричное число, пробиваемое по первому адресу).

б) ПРРД - признак режима работы программы ЗДЛ (восьмеричный код).

ПРРД = 0 00 0001 0000 0000 - режим записи информации с перфокарт на НМЛ с последующей выдачей ее на АЦПУ.

ПРРД = 0 00 0000 0001 0000 - режим записи информации с перфокарт на НМЛ без выдачи на печать.

ПРРД = 0 00 0000 0000 0001 - режим печати записанной ранее информации с помощью АЦПУ.

Для каждого записываемого файла данных задается:

в) информация к подводу очередного сектора НМЛ

0 00 НС ($\dot{i}$) 0000 0000,

где НС ($\dot{i}$) - восьмеричное число, пробитое по первому адресу, три младших разряда которого образуют номер сектора ленты, куда должен быть записан очередной $\dot{i}$ -й по порядку файл с данными ($1 \leq \dot{i} \leq$ ЧФ), а четвертый старший разряд отводится под программный номер магнитофона.

Для каждого следующего файла, подлежащего записи, данные пункта "в" повторяются.

5. Контрольная сумма исходной информации для работы.

Затем для каждого записываемого файла данных задается:

6. Колода карт с информацией i -го файла, который должен быть записан в очередной сектор МЗЛ. В конце файла (перед последней контрольной суммой) ставится признак конца файла

4 00 0000 0000 0000

Для каждого следующего файла, подлежащего записи, подкладываются данные, указанные в пункте 6.

Колода перфокарт любого приготовленного для записи файла ядерных данных делится на массивы по 320 карт. Каждый такой массив заканчивается контрольной суммой. В последнем массиве файла может быть любое, не превышающее 320, число перфокарт. В конце этого последнего массива, перед его контрольной суммой, подкладывается признак конца файла.

Ввод и запись колоды карт файла происходит массивами с выходом на "Останов" после записи каждого очередного массива. Переход на ввод следующего массива производится нажатием кнопки "Пуск". В случае сбоя массив еще раз ставится в читающее устройство и производится повторное нажатие кнопки "Пуск". Такая процедура организации записи данных на ленту менее критична к работе вводных устройств и в некоторых случаях оказывается оптимальной.

ЛИТЕРАТУРА

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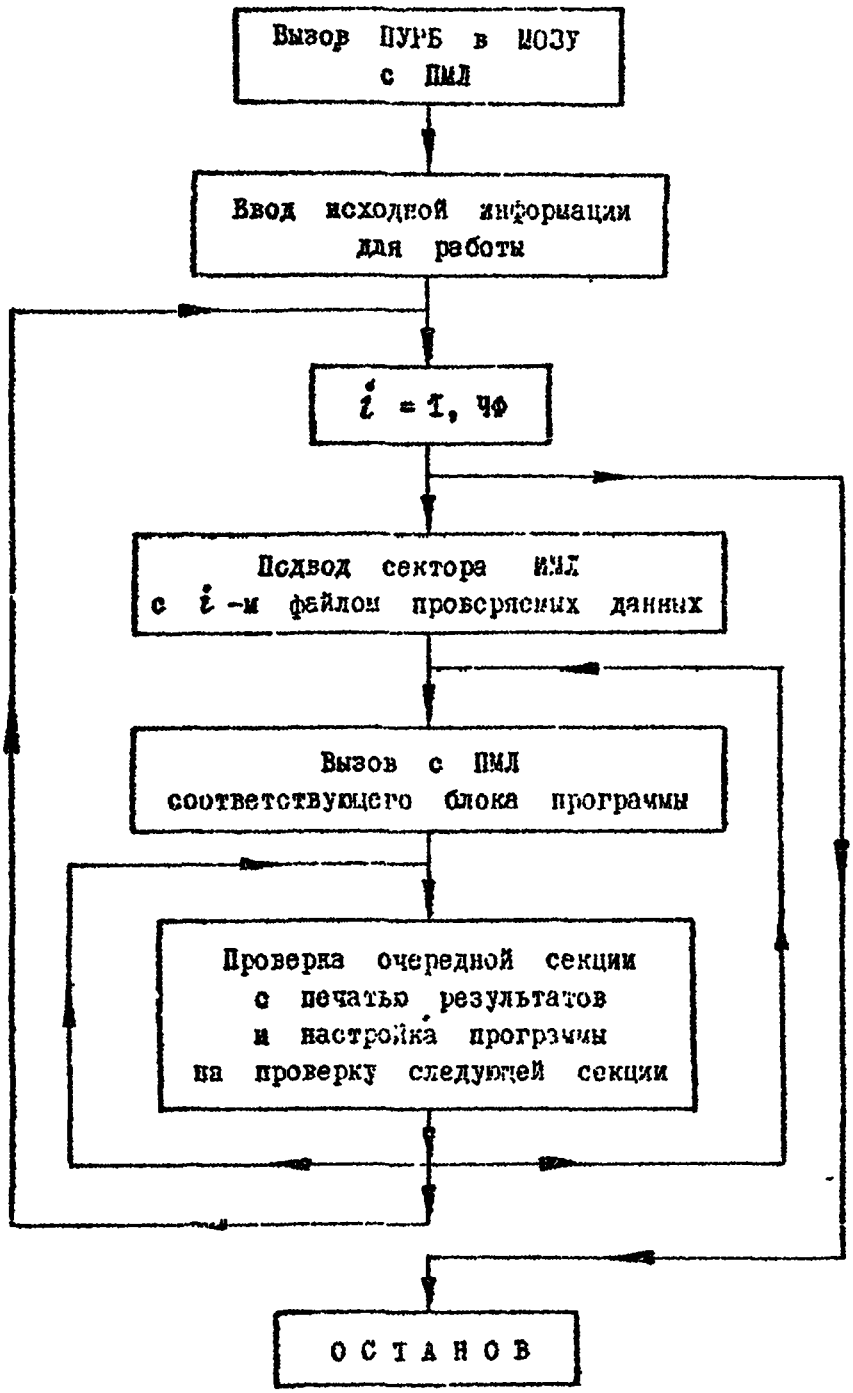
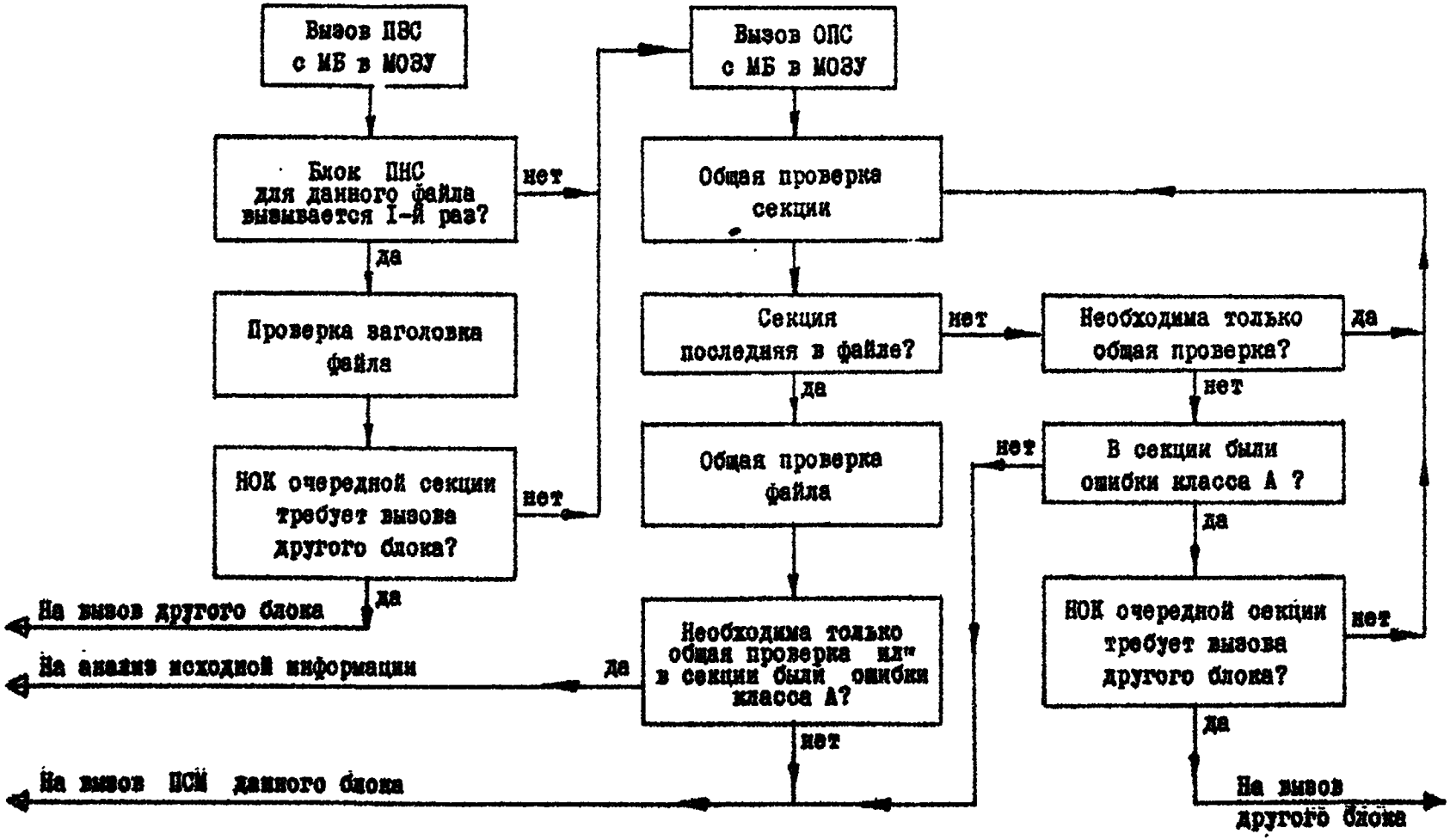
ПРИЛОЖЕНИЕ I

БЛОК-СХЕМА ПРОГРАММЫ «ПОСОЛОК»

Общая блок-схема работы программы



Блок-схема работы подпрограмм ПЗС и ОПС



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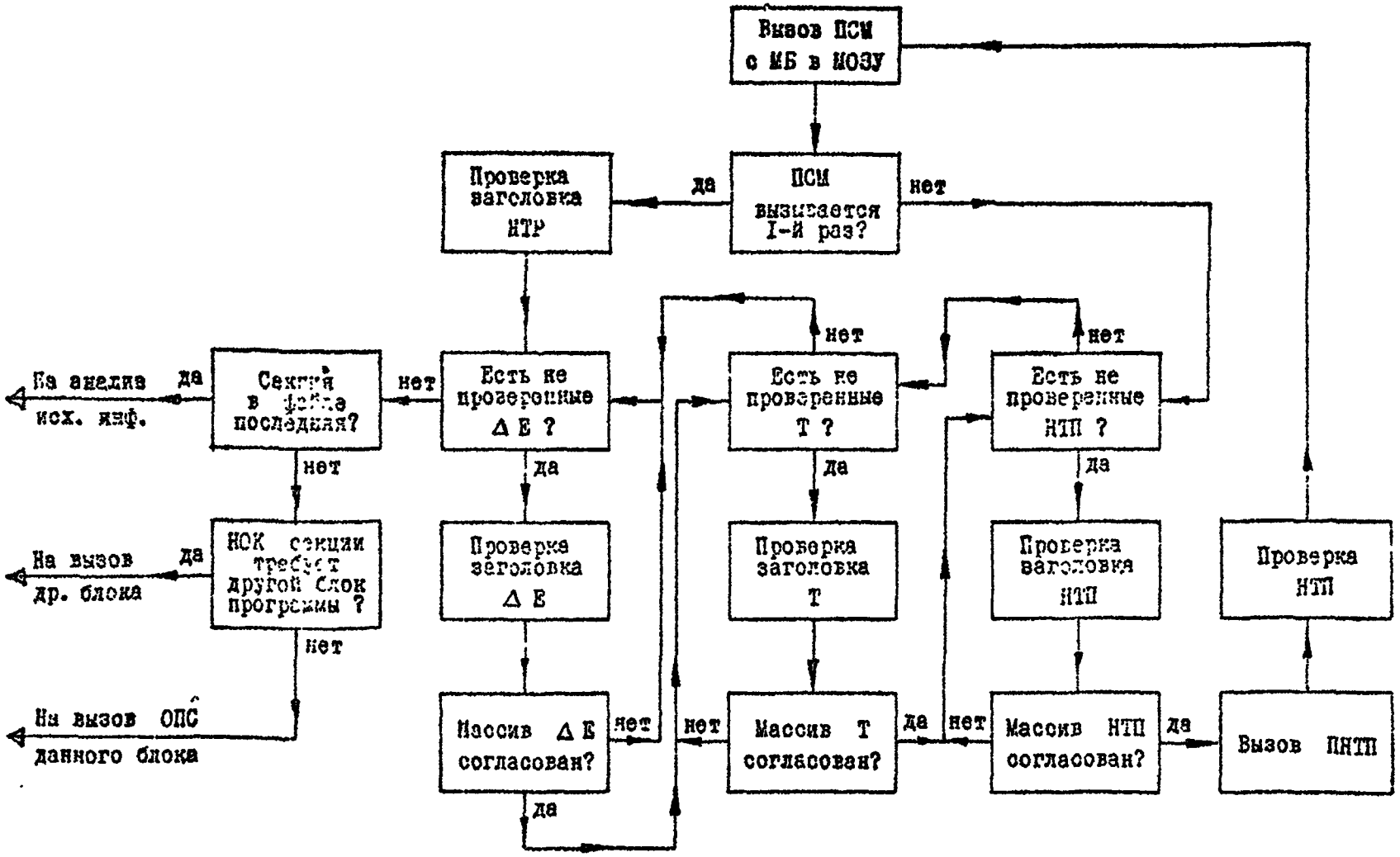

Annexes II and III

Note A detailed listing of the programme, POSOSHOK, has not been included in Annex II since some parts were not legibly reproducible. However, upon request, the IAEA Nuclear Data Section can supply copies of the listing as well as copies of Annex III, in which an example of the Print-Out is given.

Comparative Analysis of Evaluated Nuclear Data Files/Philosophy

by
S. Yiftah
Israel Atomic Energy Commission
Soreq Nuclear Research Centre, Yavne, Israel

Abstract

The paper outlines the steps which will be undertaken in performing a comparative analysis of four evaluated neutron data libraries, UKNDL, ENDF/BI, ENDF/BII and KEDAK. This study is aimed at shedding some light on the basic problem of whether the physics parameters of the fast breeder reactors presently being designed are a function of the specific evaluated data file used in the calculations. The types of comparative analysis which will be undertaken in this study are summarized.

In the framework of a scientific cooperation with the Karlsruhe nuclear research centre on "Special Topics in Fast Reactor Physics", a study has been undertaken on a comparative analysis of several relatively available evaluated nuclear data files. For the time being, the American ENDF/B I and ENDF/B II, the German KEDAK and the British UKNDL files will be studied and compared. Later, other files could be included in the study.

These basic evaluated nuclear data files of the various countries serve as the major source of input for the calculations in the framework of the big and expensive fast reactor programs. Now every country uses naturally its own evaluated file and the question that comes to mind immediately is the following: Are the physics parameters of the fast reactors being calculated and designed a function of the specific evaluated data file that is used in the calculations? In other words, would these physics parameters remain the same were the calculations to use as input a different evaluated data file?

The above mentioned study has been undertaken to try and shed some light on this problem.

Following several discussions on how to usefully tackle the problem of comparing different evaluated files, the philosophy which has evolved aims at performing the comparative analysis on several levels, namely

a) Comparison of selected important basic microscopic data of the files (for instance $\bar{\sigma}_f$, $\bar{\sigma}_{n,\alpha}$, $\bar{\sigma}_{n,n'}$, $\bar{\sigma}_{n,n''}$, of ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{238}U, ^{235}U, $\bar{\sigma}_{n,n}$ and $\bar{\sigma}_{n,n'}$, of Na and Fe to be extracted from the file and plotted, by the computer, so as to show on the same graph for certain energy ranges the data of the different files. Analysis, if possible, of the sources and reasons of the differences).

b) Comparison of the multigroup sets obtained from the basic evaluated files using the same techniques and the same averaging fluxes. This will be done for, say, 26 groups and also possibly for few groups for two and three dimensional calculations.

c) Comparative analysis of the physics parameters of three different systems, namely critical-assembly size systems prototype-size systems and 1000 Mwe-size systems.

The first critical-assembly size systems will enable comparative analysis between the different files and also between the calculated and experimental results.

The prototype-size systems, of about 3000-liter cores, will be systems typical of the several prototype fast reactors being built today (British 250 Mwe PFR, French 250 Mwe Phenix), or to be built in the future. (German-Benelux American and Japanese prototypes)

The 1000-Mwe size systems, of about 6000-7000 liter cores, are typical of the target 1000 Mwe fast power reactors being designed today by the major countries having an active fast reactor program.

The three types of systems will be calculated using the same multigroup codes with the different multigroup sets as input. The calculations will be performed in two steps:

1) One-dimensional 26-group computations using "appropriate" spherical models of the actual systems;
2) Two-dimensional 5-group and possibly 26-group computations of the same systems.

The physical parameters to be computed are: critical masses, reaction rates (ZPR's), breeding ratios, Doppler coefficients, sodium void coefficients. Other physical parameters could be added later.

Preliminary Graphical Analysis of selected plutonium isotopes cross sections of the ENDF/B-I and II, KEDAK and UKNDL files

by
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Soreq Nuclear Research Centre, Yavne, Israel

Abstract

Within the framework of the comparative analysis of evaluated neutron data libraries, the paper presents preliminary graphical results for a few important cross sections of fast reactor materials obtained from the UKNDL, KEDAK, ENDF/B I and ENDF/B II libraries.

In the framework of a general comparativw analysis of evaluated nuclear data files[1] a preliminary attempt has been done to look at the comparison of the files on the first level of microscopic cross sections.

A few pertinent cross sections of fast reactor materials in the range 0.1 to 10 Mev have been chosen for this preliminary comparison.

In order to read the ENDF/B I and II, KEDAK and UKNDL special formats, four computer programs have been prepared. To each program was added an identical subroutine for plotting the results by the computer Calcomp plotter. Each of the four programs can plot all the smooth cross sections of all the isotopes present on its library tape in a single run.

The semilog scale was found to be the best tool for comparison. Strictly speaking, this is not the right procedure for the UKNDL File which was prepared for linear extrapolation on a log-log scale. However, the data points are close enough to permit the semi-log graphical comparison. For the ENDF/B we chose a small constant lethargy step (small enough not to be recognized on the graph) and computed the cross sections at each lethargy according to the proper extrapolation scheme given by the library.

The elastic scattering, fission and capture cross sections of ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu in the energy range 0.1 to 10 Mev as plotted by the computer's plotter from the evaluated files are shown on figures 1-12.

A few preliminary remarks follow:

^{239}Pu

KEDAK calculates σ_{el} as the difference between σ_t and all other cross sections. The ENDF/B II data include the calculation of Prince (BNL) using Jupiter and Abacus-Nearrex optical model codes.

^{240}Pu

σ_f: Davey's (2) revised curve for ^{235}U has altered the ^{240}Pu fission cross section in the Mev region, as can be seen especially on the ENDF/B II curve above 6 Mev.

σ_c: In the region $0.1 < E < 0.8$ Mev, the difference is due to the use of different statistical models.

In the region $0.8 < E < 1.3$ Mev, the difference must be the result of the fast rise of σ_f (^{240}Pu threshold).

^{242}Pu

No new measurements were published in the years 1967-1970, so there is no change in the ENDF/B II with respect to ENDF/B I curves.

σ_f: ENDF/B I follows the results of Butler(3) evaluated by Davey(4) up to 1.7 Mev. Above this energy it follows ^{240}Pu as recommended by Davey.

KEDAK takes the same approach up to 1.7 Mev. Above this energy it follows exactly the ^{240}Pu fission cross section.

σ_{el}: While KEDAK follows the σ_{el} curve of ^{238}U, ENDF/B I uses deformed optical model calculations. There are no measured points in this energy region.

σ_c: The difference in the two curves is due to the use of different statistical models.

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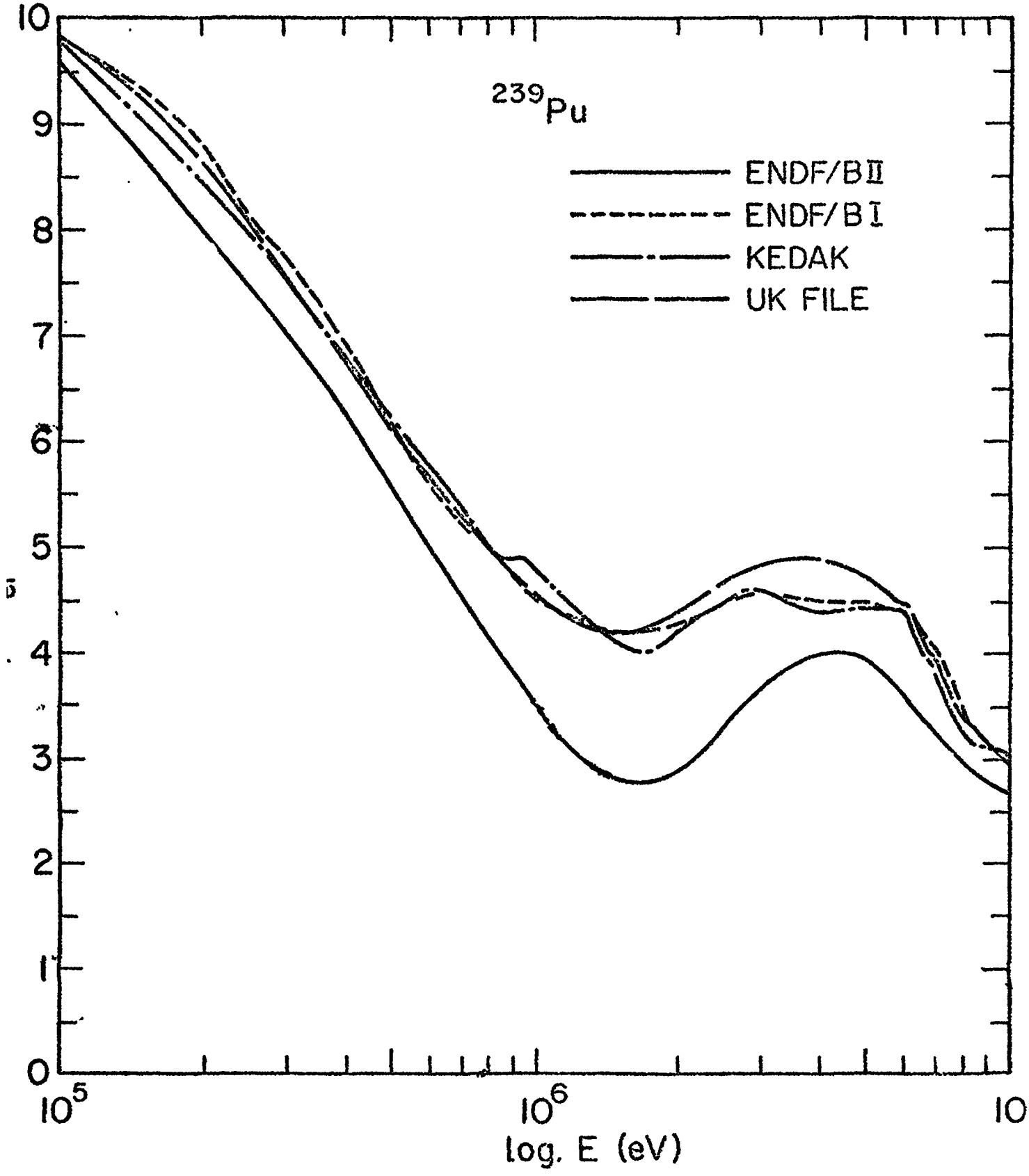
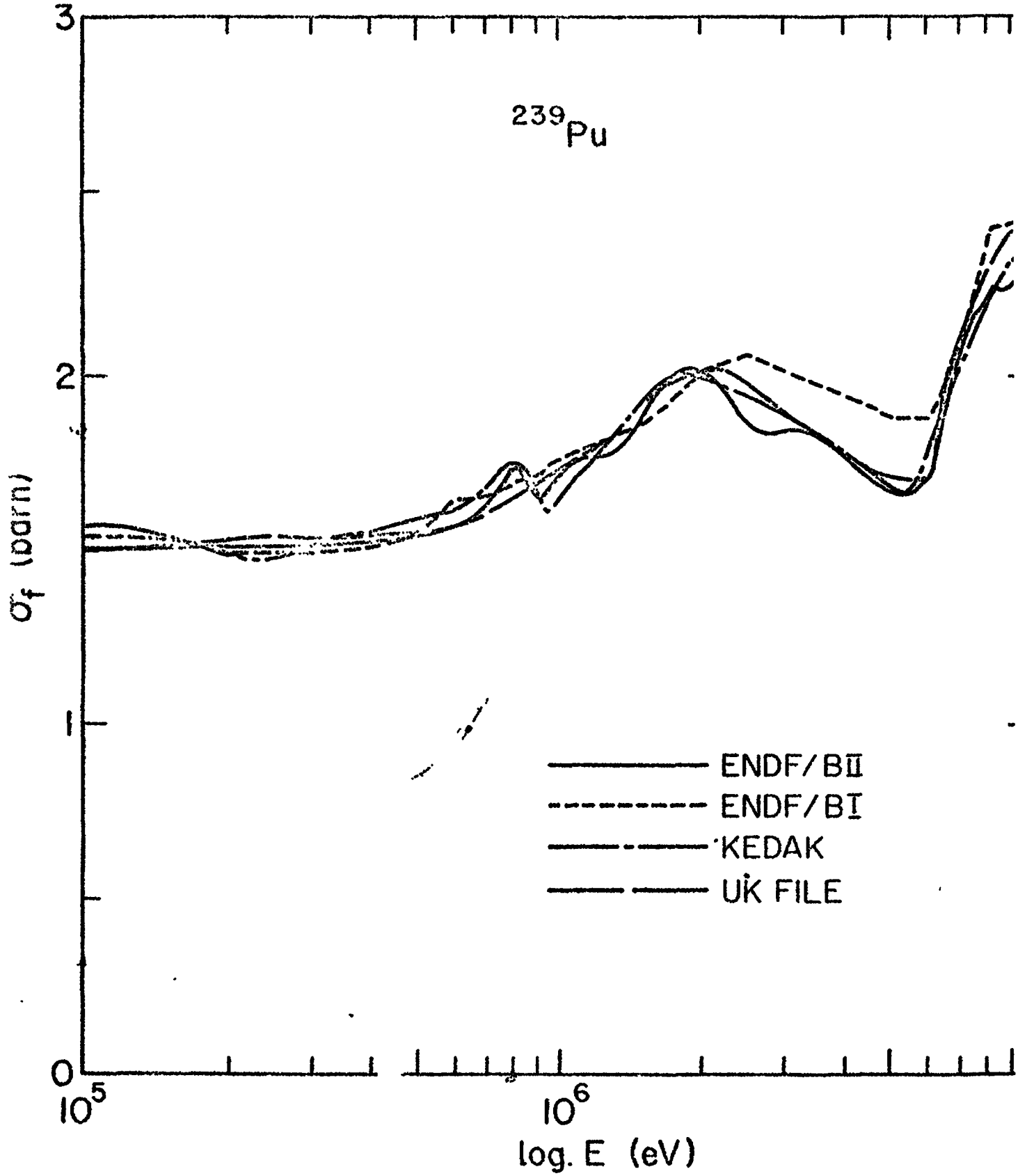
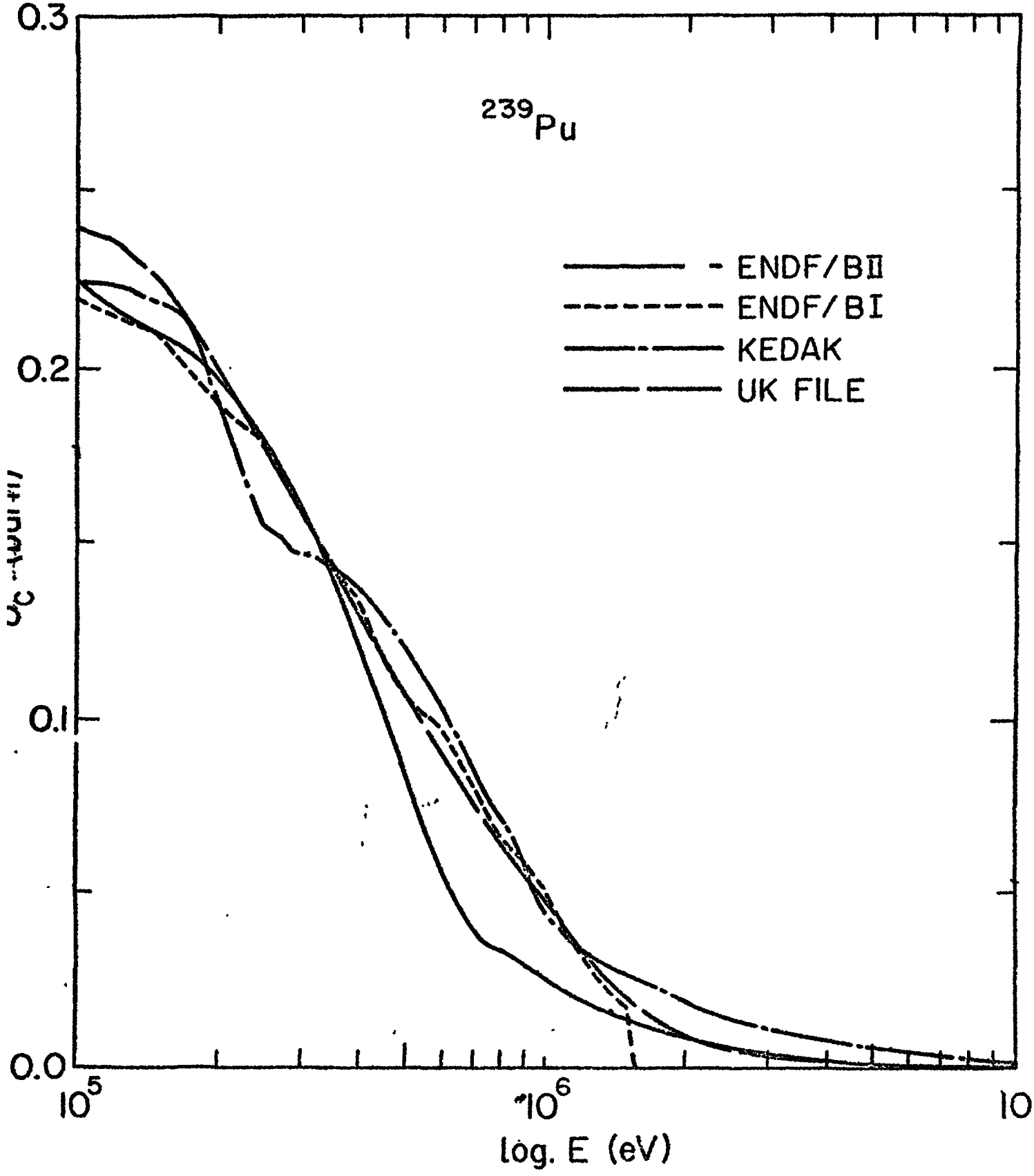
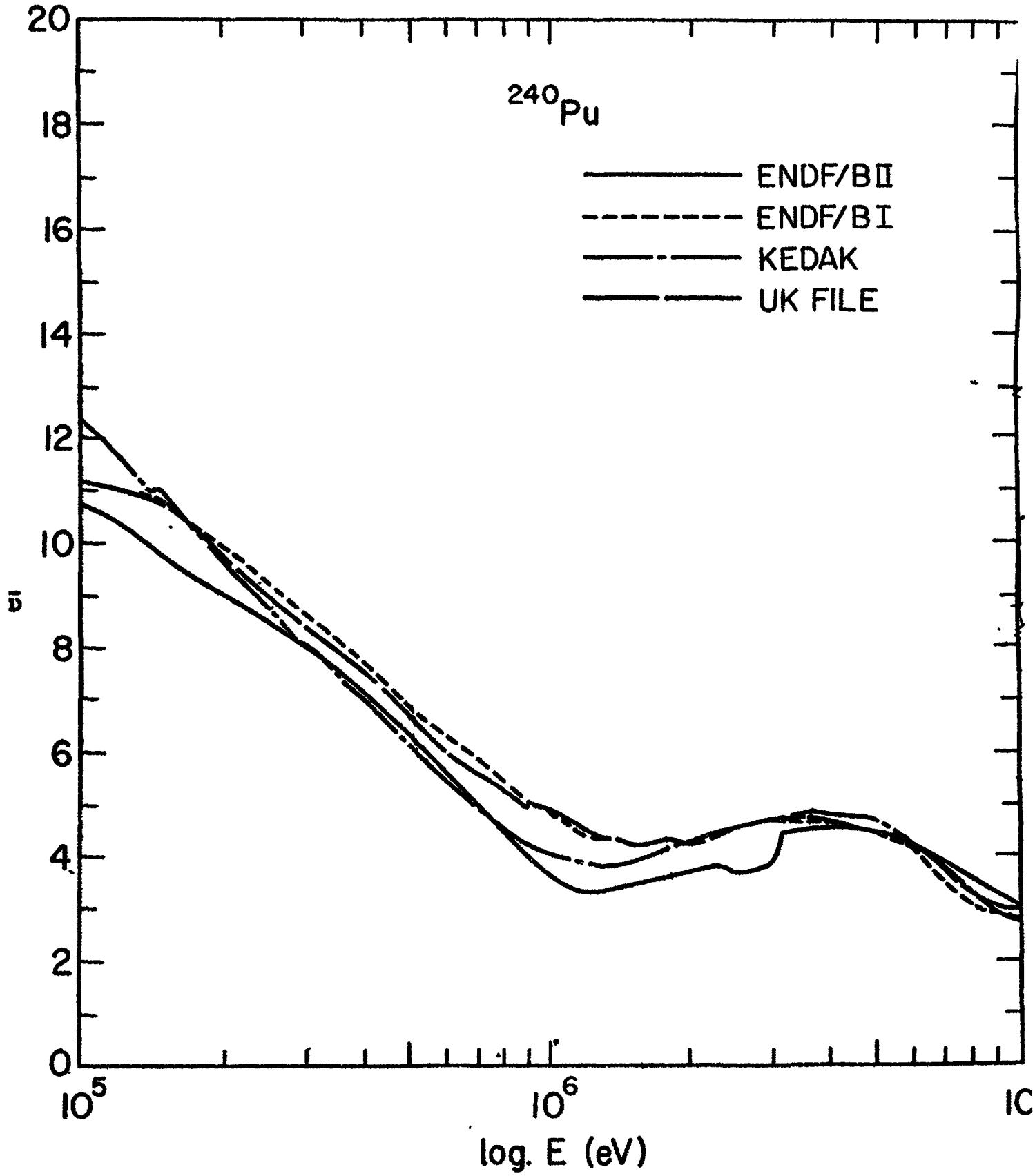
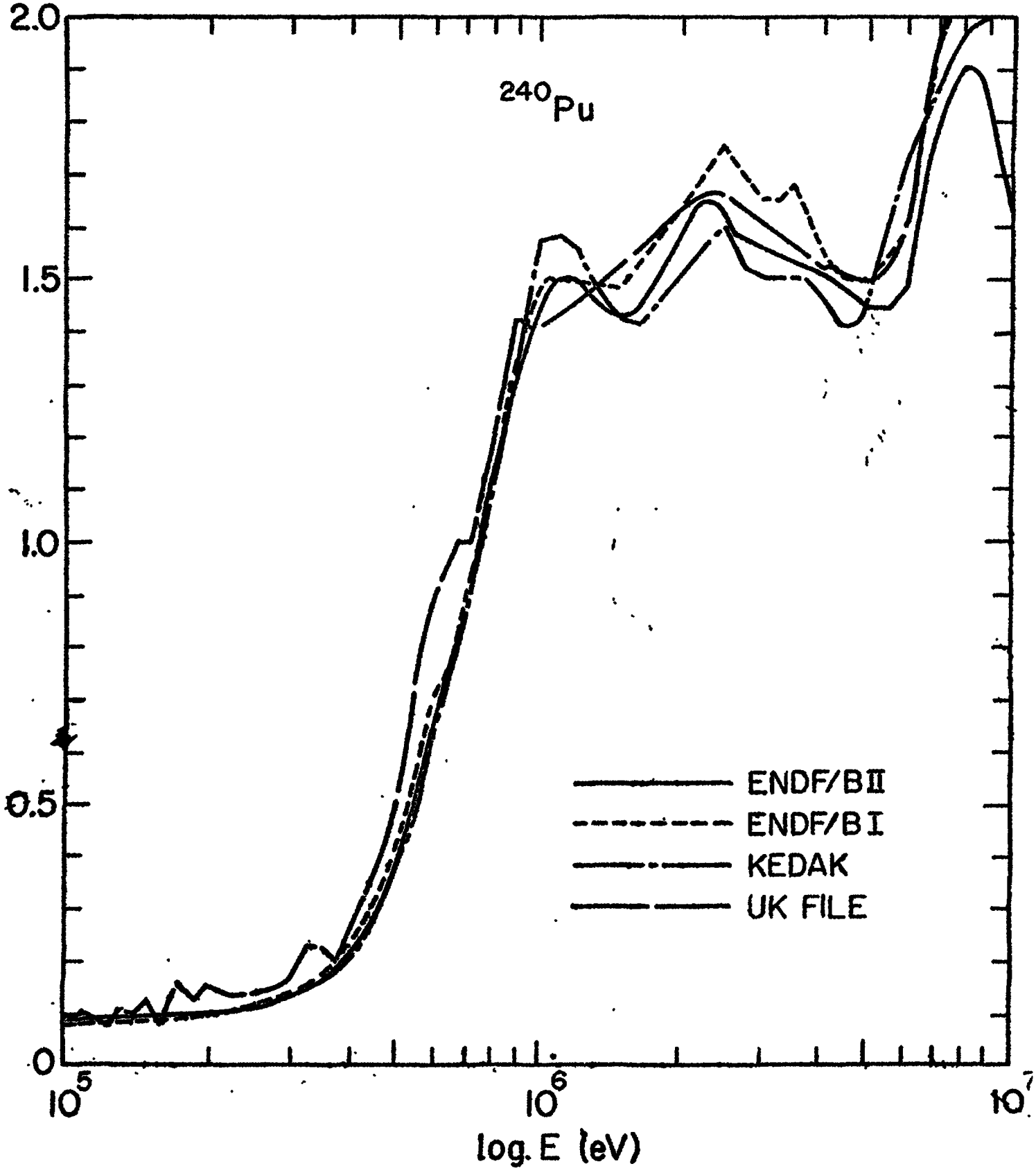
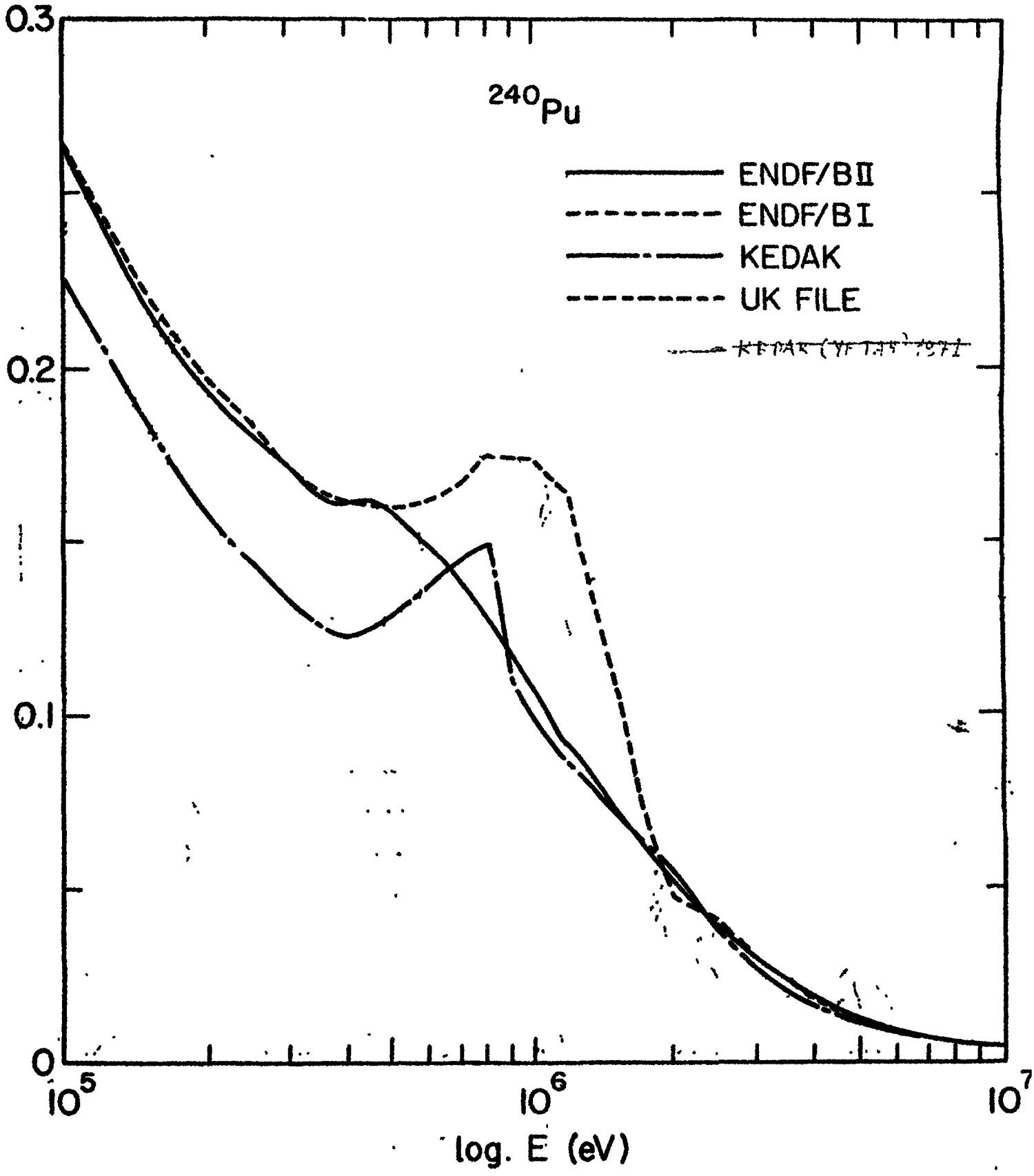

^{239}Pu
ENDF/B II
ENDF/B I
KEDAK
UK FILE
$\bar{\nu}$
log. E (eV)
10
9
8
7
6
5
4
3
2
1
0
10^5
10^6
10

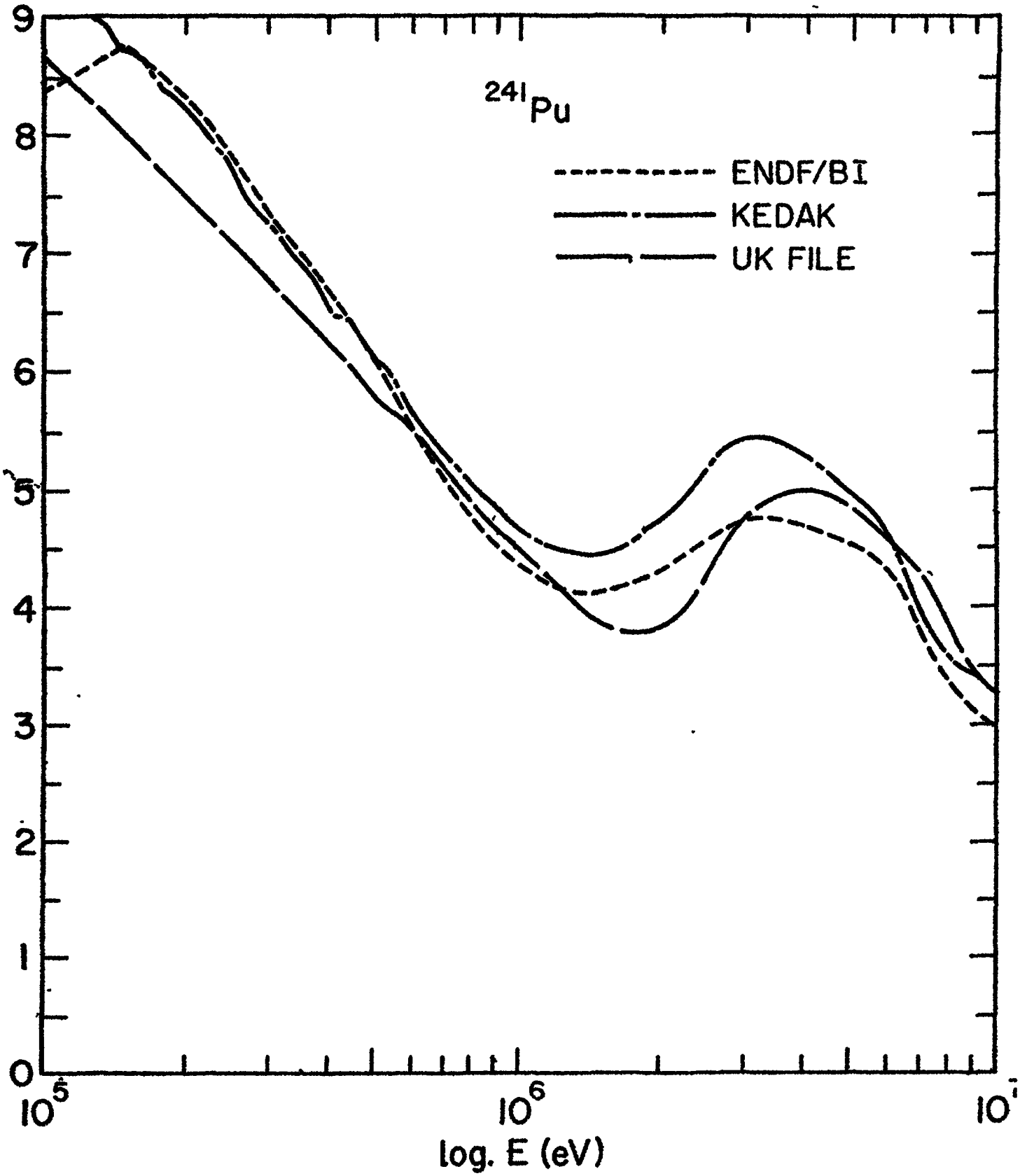

^{239}Pu
3
2
1
0
σ_f (barn)
10^5
10^6
log. E (eV)
ENDF/BII
ENDF/BI
KEDAK
UK FILE

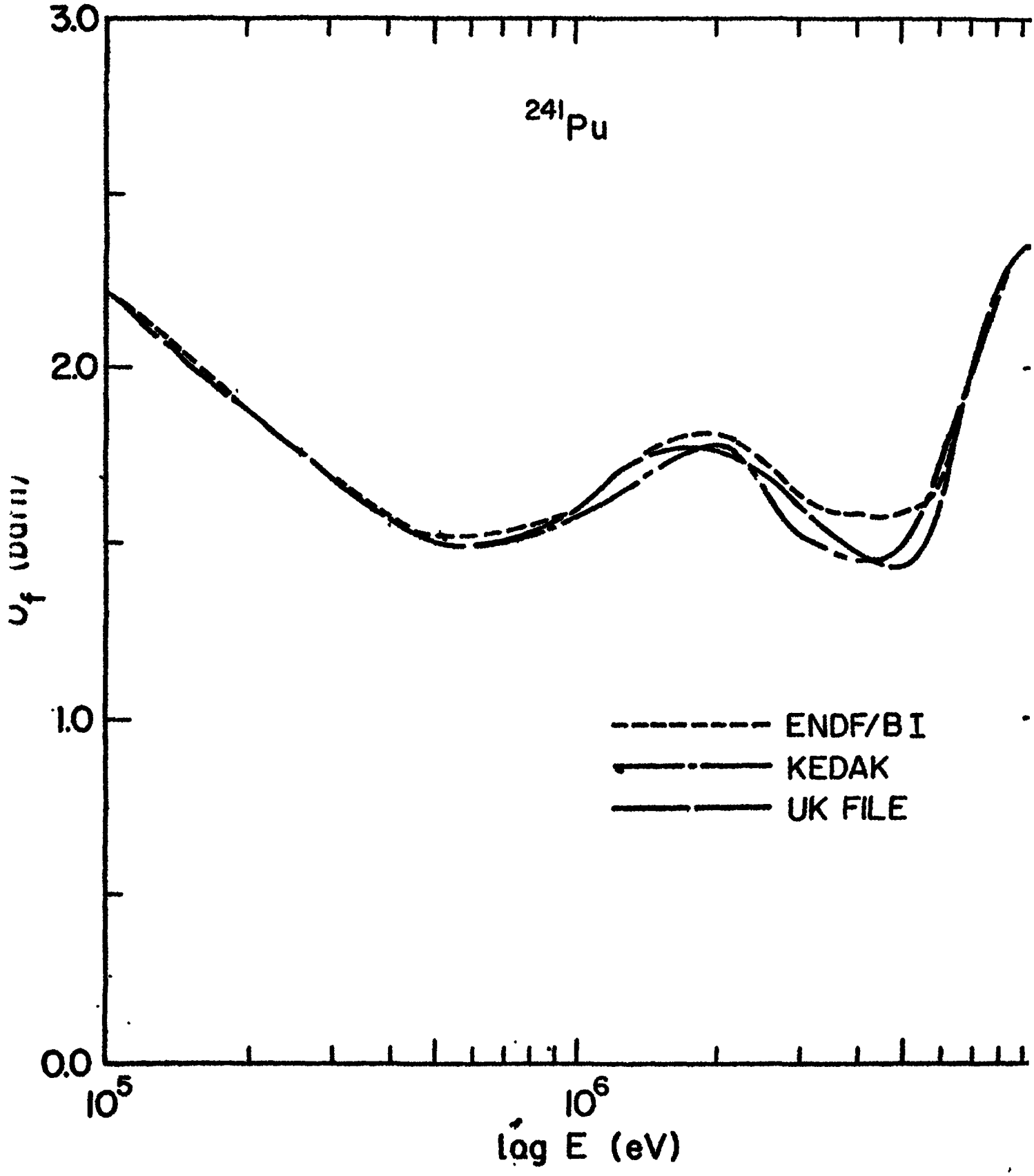

0.3
0.2
0.1
0.0
^{239}Pu
ENDF/BII
ENDF/BI
KEDAK
UK FILE
10^5
10^6
10
log. E (eV)

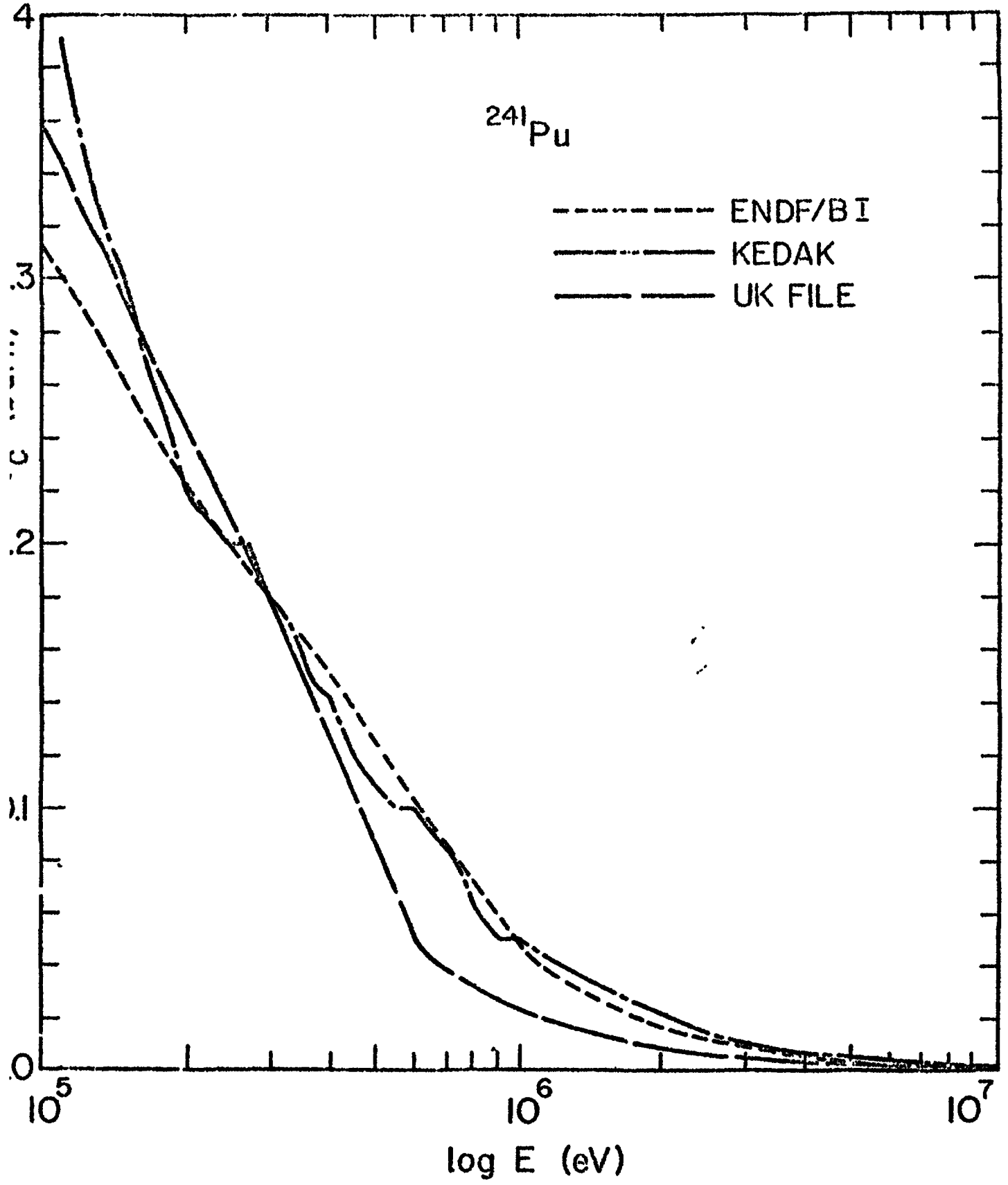

^{240}Pu
ENDF/BII
ENDF/BI
KEDAK
UK FILE
$\bar{\nu}$
log. E (eV)
20
18
16
14
12
10
8
6
4
2
0
10^5
10^6
IC

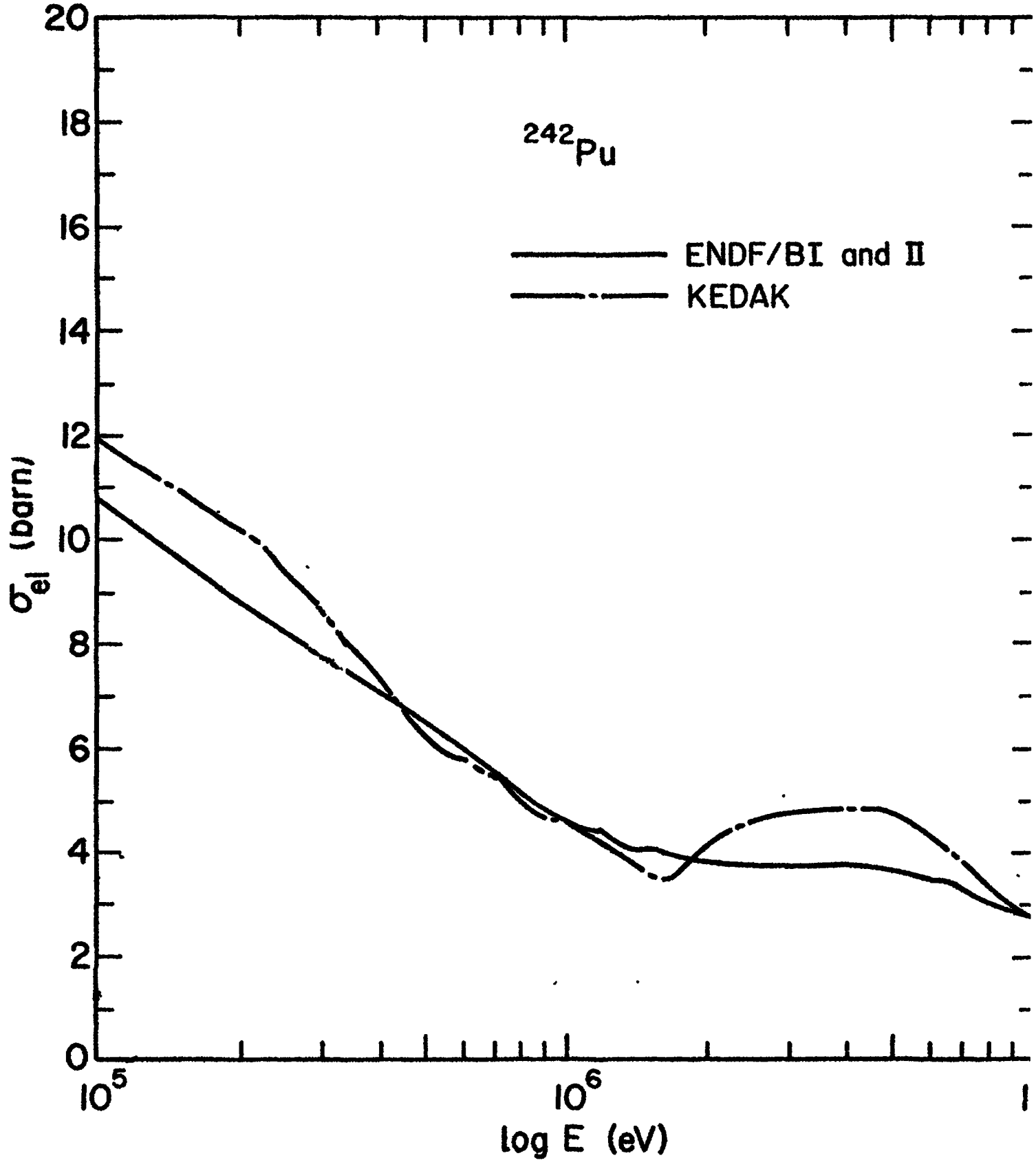

2.0
1.5
1.0
0.5
0
^{240}Pu
ENDF/BII
ENDF/BI
KEDAK
UK FILE
10^5
10^6
10^7
log. E (eV)

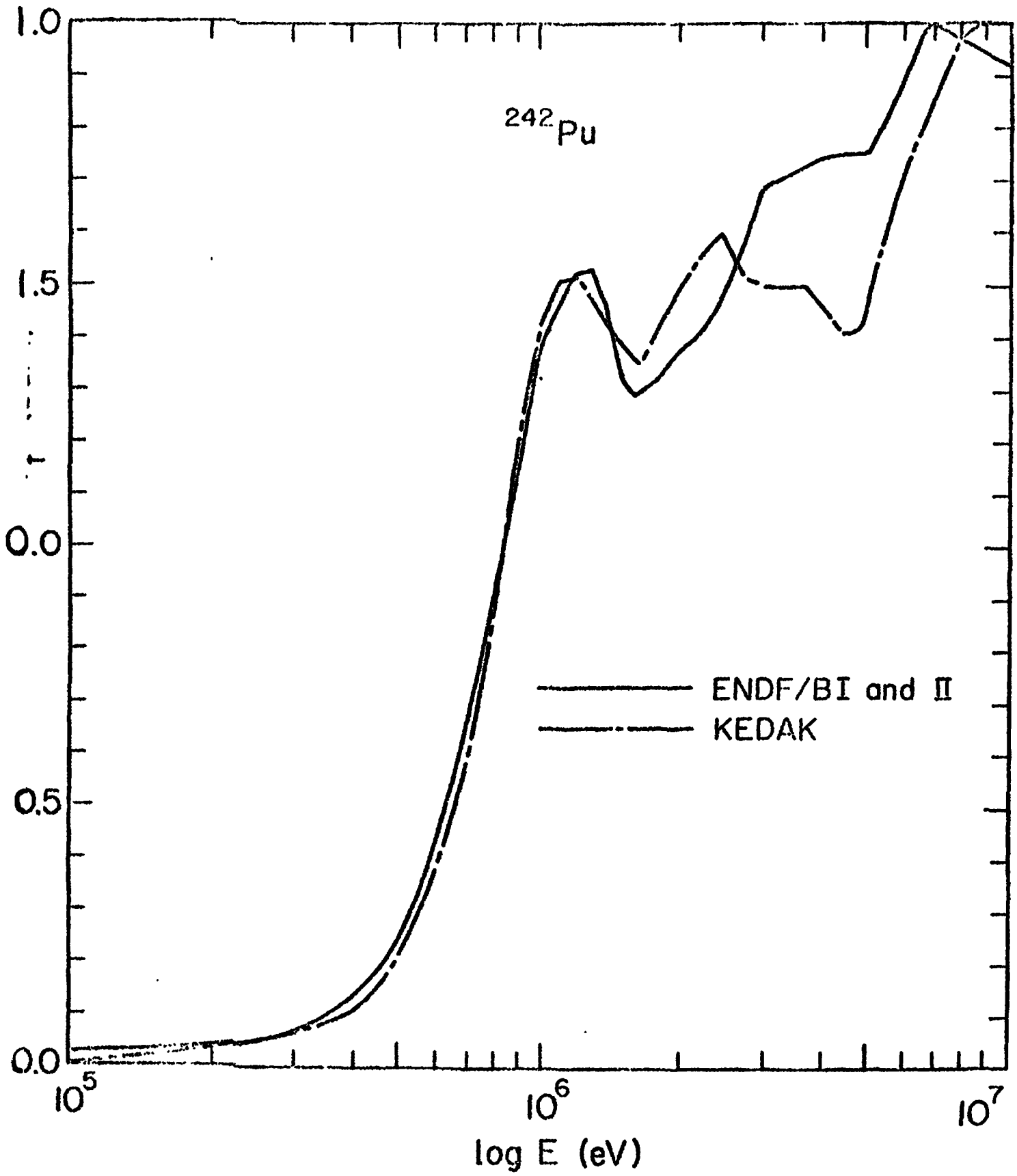

0.3
0.2
0.1
0
^{240}Pu
ENDF/BII
ENDF/BI
KEDAK
UK FILE
10^5
10^6
10^7
log. E (eV)

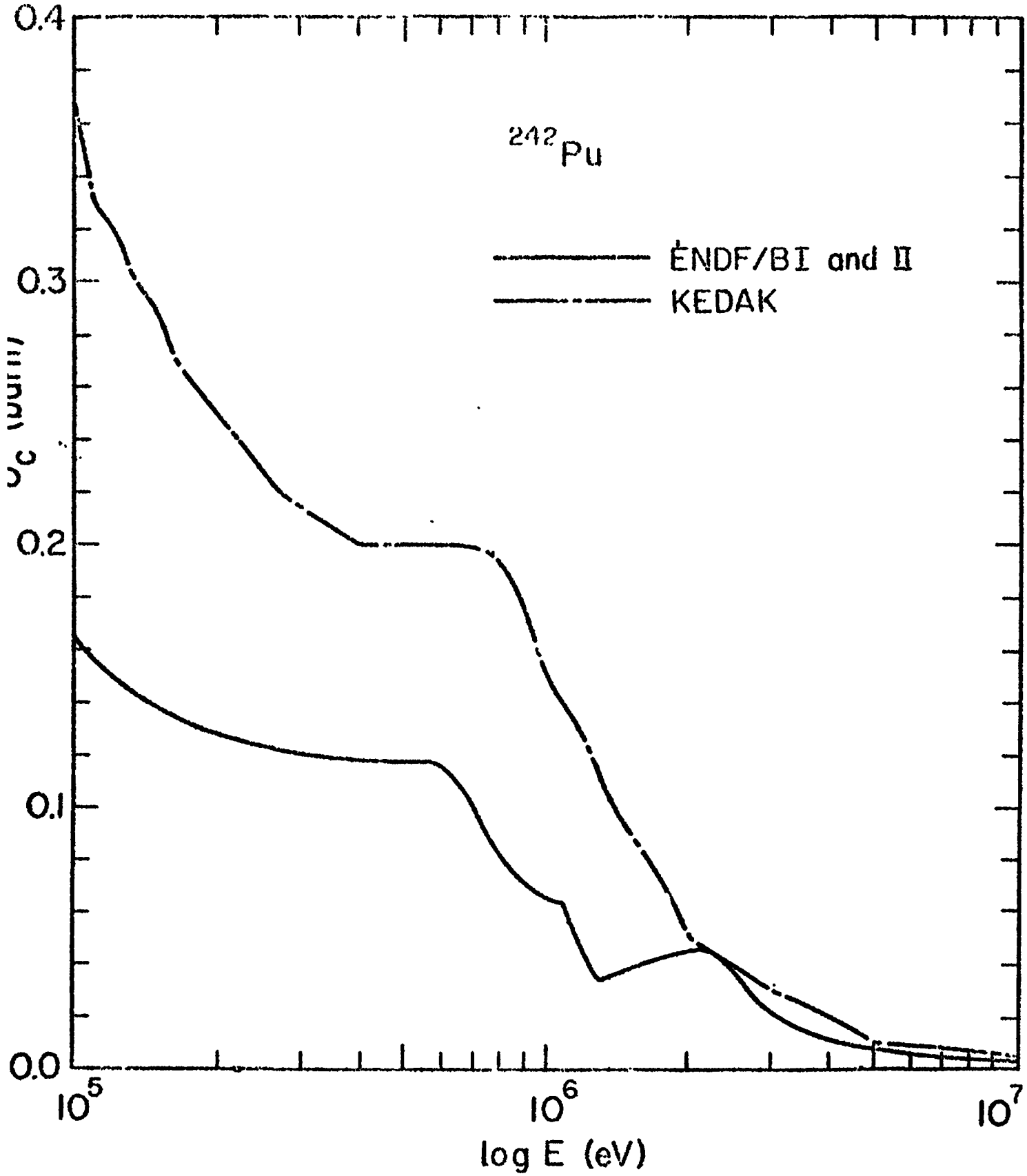

^{241}Pu
ENDF/BI
KEDAK
UK FILE
9
8
7
6
5
4
3
2
1
0
10^5
10^6
log. E (eV)


3.0
2.0
1.0
0.0
^{241}Pu
ν_f (watts)
ENDF/B I
KEDAK
UK FILE
10^5
10^6
log E (eV)


^{241}Pu
ENDF/B I
KEDAK
UK FILE
4
.3
.2
.1
0
10^5
10^6
10^7
log E (eV)


20
18
16
14
12
10
8
6
4
2
0
σ_{el} (barn)
^{242}Pu
ENDF/BI and II
KEDAK
10^5
10^6
1
log E (eV)


1.0
1.5
0.0
0.5
0.0
^{242}Pu
ENDF/BI and II
KEDAK
10^5
10^6
10^7
log E (eV)


0.4
0.3
0.2
0.1
0.0
^{242}Pu
ENDF/BI and II
KEDAK
10^5
10^6
10^7
log E (eV)

THE ROLE OF PHYSICAL TRENDS IN NEUTRON DATA EVALUATION

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Debrecen, Hungary

Different trends and tendencies are surveyed for /n,total/, /n,2n/, /n,γ/, /n,p/ and /n,α/ cross sections with special emphasis on the first two cases. The observation and interpretation of such trends has great scientific interest and can serve as a guide in checking these data; also, it can be used in the estimation of cross section values that have not been measured. For /n,total/ cross sections no definite odd-even and N-Z effects were observed; the existence of a fine structure for light nuclei was established and described by a simple formula /"binding energy effect"/. In the case of /n,2n/ cross sections at constant excess energy above threshold there exists a definite N-Z dependence. The odd-even and shell effects observed previously, are mainly due to the threshold energies.

INTRODUCTION

For fast neutrons most of the cross section measurements can be found around 14 MeV. Previous investigations [1-17] of cross section systematics for /n,total/, /n,2n/, /n,γ/, /n,p/ and /n,α/ processes suggest that shell structure, N-Z symmetry

parameter, odd-even and mass number effects exert a strong influence on the data at 14 MeV. The observation and interpretation of tendencies in the cross sections has not only scientific interest: such tendencies can serve as a guide in checking the reliability of the data and in estimating cross section values that have not been measured. At present according to our survey of fast neutron reaction cross sections, only about 30 per cent of the measurable data are known. The great number of unknown data can be explained by the unfavourable decay schemes because the reaction cross sections have been measured with a few exception by activation method. The lack in data and the gross disagreements among the existing data make more difficult the revealing of tendencies and checking the applicability of nuclear theories. More detailed trends can only be revealed from data measured by the same author where the relative accuracy is higher. Using up-to-date values, a review is given on some tendencies in total and reaction cross sections and their role in the evaluation of cross section data.

TOTAL NEUTRON CROSS SECTIONS

Among fast neutron data the total cross sections are the most complete and accurate, so they give reliable information on the average properties of nuclei. Furthermore it seems worth while to search for such systematic behaviour in

total cross sections as have been found in reaction data. In our investigations at 14 MeV total cross sections were measured under the same circumstances to improve the relative accuracy, and the best averages of literature data for the 13-15 MeV interval were calculated using a statistical procedure [18].

In our experiments the choice of the samples was subordinated to the aim of observing possible N-Z or odd-even effects. E.g. to check the N-Z dependence, the A-Ca isobaric pair were measured, too. Though for some pairs significant deviations were observed, these can not be definitely attributed to odd-even or N-Z effect.

In order to search for fine structure in the mass number dependence of the cross sections, the experimental data were divided by the black nucleus formula, accepting $r_0 = 1.4$ f, $\lambda = 1.22 \frac{A+1}{A}$ f and $R = r_0 A^{1/3}$.

The results are shown in Fig.1. /crosses: present work, circles: averages of literature data/.

As it can be seen, the reduced cross section values show a sinusoidal form in the function of $A^{1/3}$.

It was found that the data in Fig.1. can be well described by the following empirical expression /dashed curve/:

$$\sigma_T \approx 2\pi(R+\lambda)^2 \left[1.02 - 0.104 \cos(2.18 A^{\frac{1}{3}} - 1.25)\right] \quad /1/$$

In general the good fit of this simple formula to

the experimental data for medium and heavy nuclei suggests that if exists any systematic trend in total neutron cross sections, superimposed on this gross structure, its magnitude does not exceed a few per cent. Expression /1/ can be used for the calculation of unknown total cross sections in the mass number region mentioned above. Similar expressions can be used also for neutron energies between 0.5 and 42 MeV; only the numerical parameters should be changed. As for light nuclei the dashed curve does not fit well to the reduced experimental cross sections although its shape is similar. As it was shown in our earlier paper [19], a correlation exists between r_o and the binding energy per nucleon. This suggests that the higher r_o values in this region are in connection with a loose nuclear structure, resulting in a higher cross section. The deviations for pairs measured can be mainly explained by the binding energy effect.

/n,2n/ CROSS SECTIONS

Various trends have been observed in /n,2n/ reaction cross sections versus mass or neutron number for 14 MeV neutrons. Barr et al. [7] observed a tendency of (N-Z)/A dependence in the ratio σ_{nM}/σ_{ne} where σ_{nM} and σ_{ne} are the neutron emission and nonelastic cross reactions, respectively. The results of Pearlstein [20] and Breunlich et al. [9] support the observation of these systematic deviations between the theoretical and experimental cross

sections as a function of (N-Z)/A as well as N-Z. Near threshold the value of the /n,2n/ cross sections strongly depend on the difference between the bombarding and the threshold energy. At a given bombarding energy the Q value markedly influences the reaction yield. For this reason it seemed interesting to examine the behaviour of /n,2n/ cross sections for a constant bombarding - threshold energy difference. The cross sections determined in this way at 3 MeV excess energy were found to differ markedly for different nuclei of the same target neutron number N, and no significant shell effect could be recognized [21]. Plotting these values against N-Z at given N or Z, the data lie on a straight line, independently of Z or N being even or odd /Fig.2/. The straight lines for different N or Z are parallel to each other in good approximation, except for N=28. This means that a simple formula can be given for calculating /n,2n/ cross sections in the interval $30 \leq N \leq 120$ investigated.

$$\sigma(Z \pm \Delta Z, N) = \sigma(Z, N) \mp m(E_{exc.})\,\Delta Z \qquad /2/$$

For $E_{exc} = 3$ MeV one finds $m/E_{exc}/ \approx 231$ mb. This empirical formula can be applied also to other energies by using the Weisskopf estimate for the energy dependence.

On the bases of the above mentioned and in the knowledge of /n,2n/ cross sections of some nuclides

data for further nuclides could be estimated by interpolation and extrapolation. Owing to the fact, that the linear N-Z dependence holds either for constant N or for constant Z, there are cases where the systematics gave the same cross sections in two independent ways. Such examples are given in Table I. in order to show the inner consistence of the systematics. Finally, the cross sections for elements have also been calculated at 14.7 MeV by averageing over isotopic abundances. As it can be seen in the Fig.3. the tendency of the original experimental data is fairly well followed by the values for which the N-Z systematics was taken into account. In the case of light nuclei the odd-even effect can be well observed; this - similarly to the shell effect - is probably caused by the variation in the threshold energies. Using the N-Z tendency, an empirical analytical expression for calculation of /n,2n/ cross sections has been given by Ádám and Jéki [22]. The agreement between measured and predicted values is fairly good for nuclei with $4 \leq N-Z \leq 21$.

/n,γ/ CROSS SECTIONS

Only a few published data are available concerning capture cross sections for neutrons above 1 MeV [10,11,23,24]. The examination of these seems to show some regular behaviour, which may suggest new indicative measurements. Most of the data refer to unmoderated fission neutrons. The

target neutron number dependence of these data shows a definite shell effect; in addition, an increase in the neutron number for $N \leq 60$ is accompanied by an increase in the neutron capture cross sections, while for $N > 60$ a saturation can be observed /Fig.4./. In order to complete existing data and to check the energy independence of the observed tendencies, further measurements at 3 and 14 MeV were carried out by activation method [25,26,27].

The measurements, especially at 14 MeV, were difficult because of the low cross section values and of the concurrent reactions. Figs. 5 and 6. show the capture cross sections at 3 MeV and 14.7 MeV as a function of target neutron number and includes the results of other published measurements. The data show a trend similar to that observed by Hughes et al. at 1 MeV. At the magic neutron numbers the cross sections are small in comparison with those of neighbouring nuclei. Cross section measurements on additional nuclei with non-magic N, performed to confirm these minima, unfortunately were not successful due to competitive /n,2n/ reactions at 14 MeV.

A decreasing trend of cross sections as a function of N-Z can be observed at a given neutron or proton number for the energies mentioned above.

The increasing trend of the 14 MeV cross sections for the N=82 nuclei Ba, La and Pr and for the N=126

nuclei Pb and Bi is similar to that found at 1 MeV. Thus the treuds observed in the /n, γ/ cross sections at 1 MeV remain valid at higher neutron energies, they seem to be independent of the number of possible reaction channels. According to our investigation the /n, γ/ cross sections are proportional to A^3 at 1, 3 and 14 MeV /see e.g. Fig.7./

Longo and Soporetti [12] plotted the logarithm of experimental /n, γ/ cross sections at 14 MeV for nuclei with proton numbers Z >28 in the function of $(N-Z)^2/A$. Cross sections for nuclei with neutrons in the same shells are on straight lines : $\ln \sigma \propto - (N-Z)^2/A$, suggesting that for a given neutron shell the /n, γ/ cross sections decrease exponentially with the increase of the parameter $(N-Z)^2/A$. /Fig.8./
Further measurements are needed to check the mentioned /n, γ/ trends.

/n,p/ AND /n,α/ CROSS SECTIONS

For fast neutron reactions most of the data refer to /n,p/ cross sections around 14 MeV. Plotting the /n,p/ values in the function of mass number Gardner [28] found that for each element the cross section of an isotope is about half of the preceding one. A semilogarithmic plot shows that the distance between lines of different elements is about the same for a wide range of atomic number. Using this,

simple empirical expressions could be given for the Z and A dependence of σ/n,p/.

$$\sigma(Z, A\pm1) \approx \sigma(Z, A) \cdot 2^{\mp1}$$
$$\sigma(Z\pm1, A) = \sigma(Z, A)\, m^{\pm1} \qquad /3/$$

where m=4.6 and m=6.6 for the light and heavy elements respectively. Another empirical formula for /n,p/ cross sections has been given by Levkovskii [16]:

$$\frac{\sigma(Z, A+\Delta A)}{\sigma(Z, A)} \approx \exp\left(-33\frac{\Delta A}{A}\right) \qquad /4/$$

Values calculated by this expression agree well with those determined by /3/.

About 80 per cent of the cross sections can be well approximated by these empirical formulae, hence they can be applied to estimate unknown data. Deviations occur mainly at closed proton and neutron shells which could be interpreted by variations in the Q-value, level density and pairing energy around the closed shells.

Analyzing /n,p/ cross sections Chatterjee [17] found that for reactions leading to magic residual nuclei, a minimum in the σ/n,p/ values should appear. Unfortunately, at those nuclei experimental data are rather scanty. Our measurements [29] lead to the following conclusions: The data obtained for the isotopes ^{45}Sc and Ca at Z_R = 20 do not confirm the proton-shell effect in the dependence of σ/n,p/ on Z_R. The applicability of the empirical formulae relating to the dependence of σ/n,p/ on the mass

number for a fixed Z were confirmed by the data measured for the nuclei $^{42,43,44}Ca$ and $^{188,190}Os$. According to our measurements, the absolute cross section values agree in all cases with those calculated from the empirical equations /16,28/ relating to $\sigma/Z,A/$ within a factor of two. The agreement is especially good in the case of nuclei $^{42,43,44}Ca$. /Fig.9./.

As for the Z dependence of /n,α/ cross section values one can conclude, that the cross sections generally decrease from $\sim$100 mb to $\sim$1 mb from the lightest to the heaviest elements. Two definite maxima can be seen, one in the region from Na to Cl /$\gtrsim$100 mb/, the other in the rare earth region /$\sim$ 10 mb/. At the magic neutron number 50 the cross sections are considerably higher than for the neighbouring nuclides. Gardner and Yu-Wen Yu [14] gave an empirical expression for /n,α/ cross sections which can be usefully applied to estimate unknown data. The agreement between measured and calculated data is not so good as in the case of /n,p/ cross sections.

The spread in the present data is caused mainly by the different experimental circumstances. Therefore it would be profitable to recommend standardized conditions for the irradiations and activity measurements using modern experimental techniques. These could perhaps be developed-under the auspices of the Agency-by the institutes that

have traditions and current work for neutron data measurements. A great number of data measured by the same method and under the same circumstances, would be of great help to check the validity of tendencies and also to investigate nuclear structure and reaction mechanism.

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Table I.

Data obtained from the N-Z trend both for constant N and Z at 3 MeV excess energy. Estimations from using isotonic and isotopic lines /independent data/ agree well with each other.

Nuclide	N = constant		Z = constant	
	σ(mb)	$\Delta\sigma$	σ(mb)	$\Delta\sigma$
Cr-54	870	70	830	130
Zn-68	1050	80	845	60
Ge-72	790	40	800	30
Mo-94	765	70	710	70
Mo-96	900	60	1030	100
Mo-98	1030	100	1320*	130
Se-78	965	40	950	40
Se-80	1160	180	1030	660
Sr-88	1300	130	1320	130
Ru-102	1060	70	1020	90
Te-130	1470	120	1310	90
Er-162	2020	200	1820	140
Sn-118	1190	80	1310	80
Hf-176	1820	120	1840	120
Hg-196	2000	150	1820	150
Sm-152	1710	170	1490	140

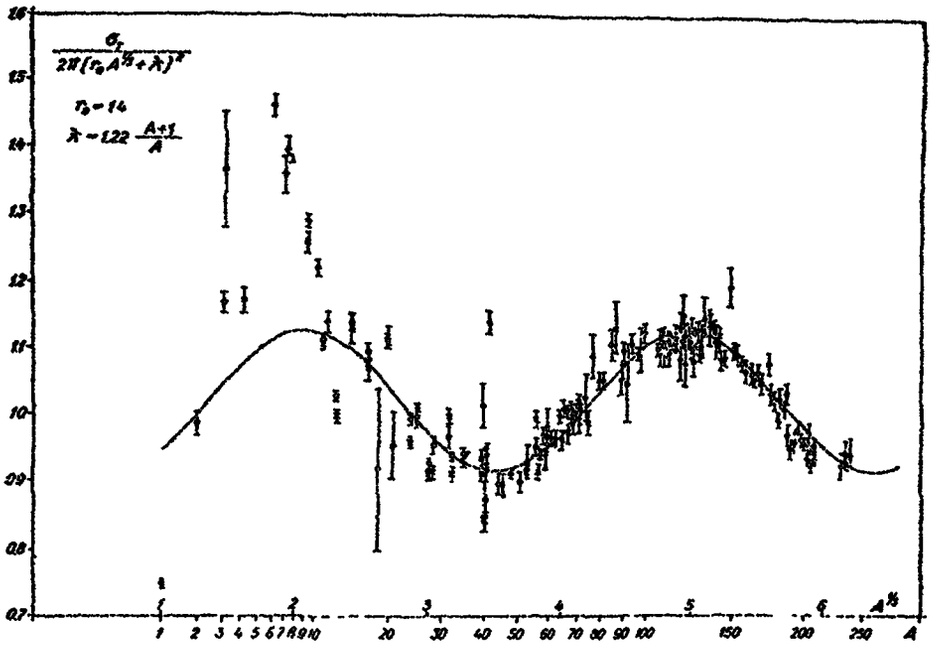

Fig.1. 14 MeV neutron total cross sections divided by $2\pi(R+\lambda\!\!\!^{-})^2$ as function of $A^{1/3}$.

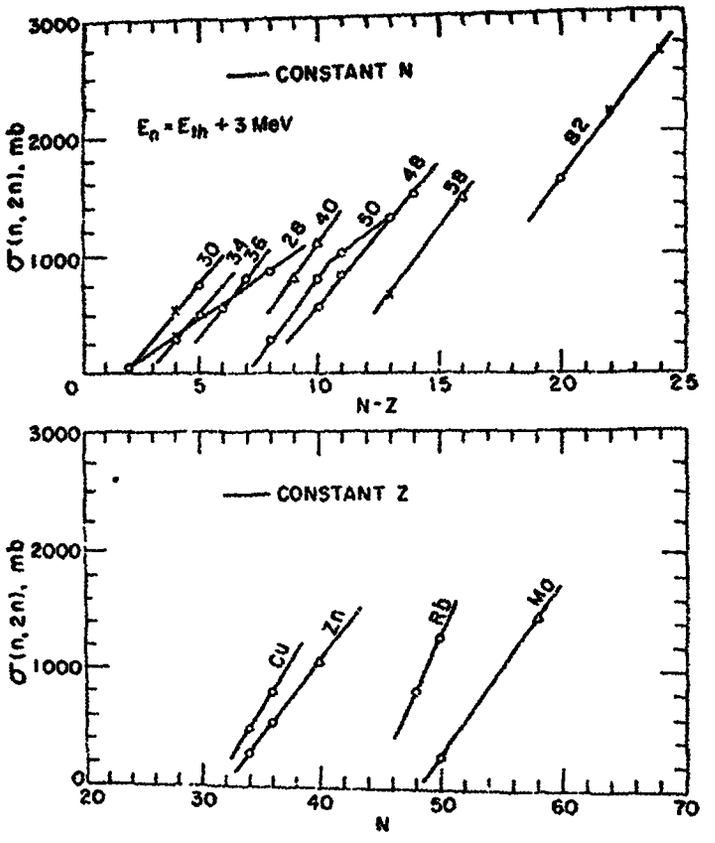

Fig.2. Systematic behaviour observed in /n,2n/ cross sections.

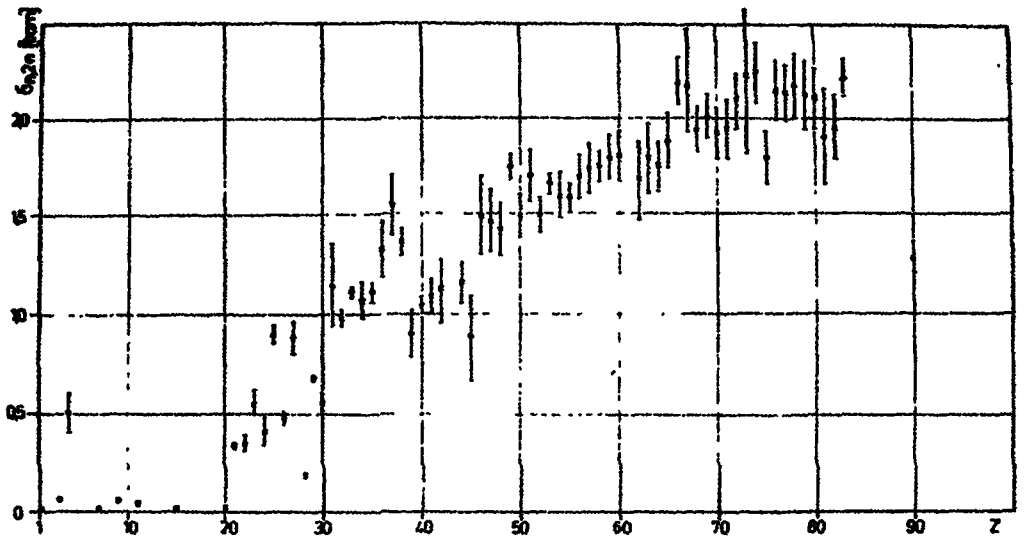

Fig.3. /n,2n/ cross sections for elements at 14.7 MeV.

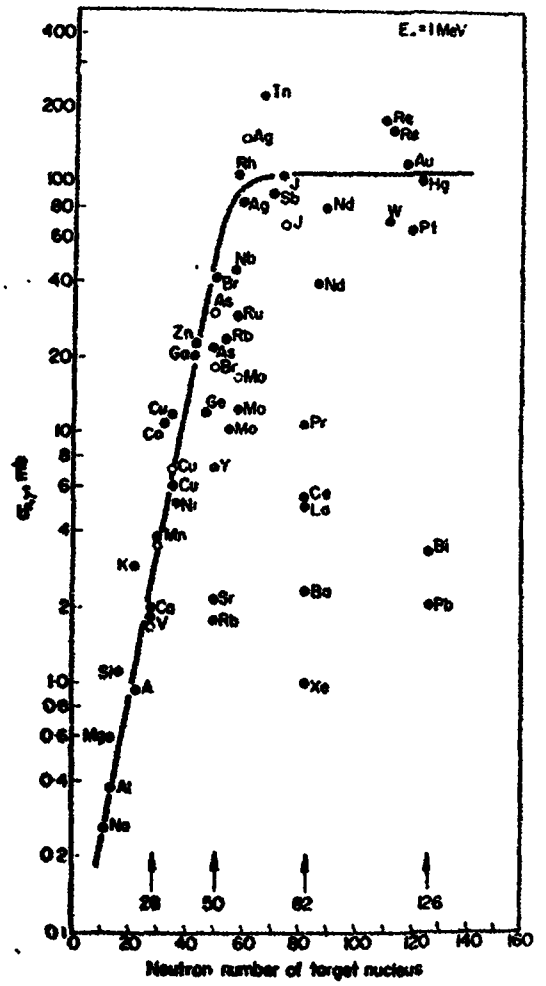

Fig.4. Radiative capture cross sections for unmoderated fission neutrons.

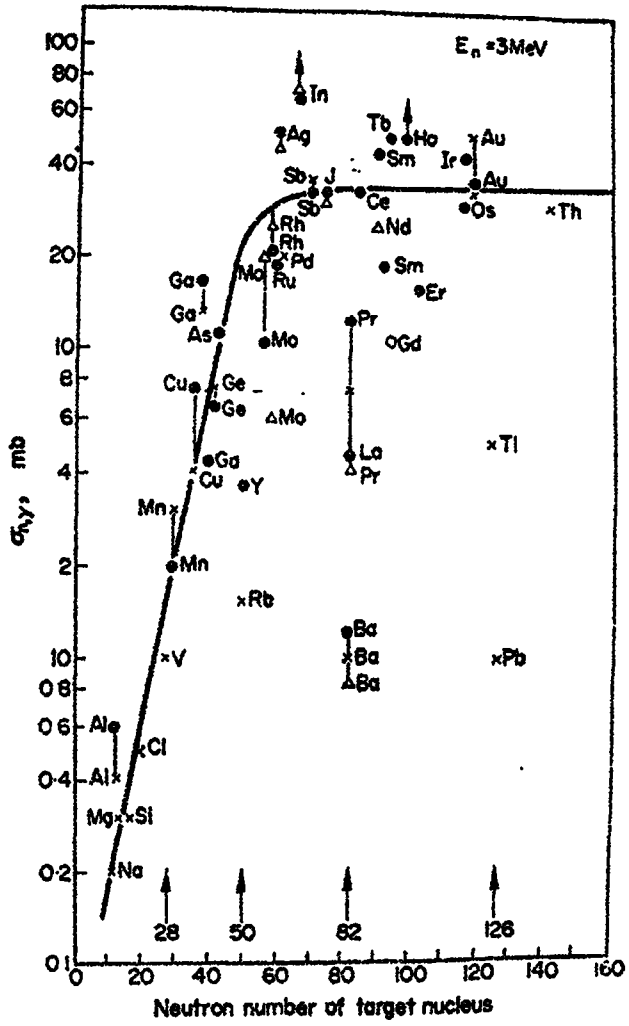

Fig.5. Radiative capture cross sections for 3 MeV neutrons.

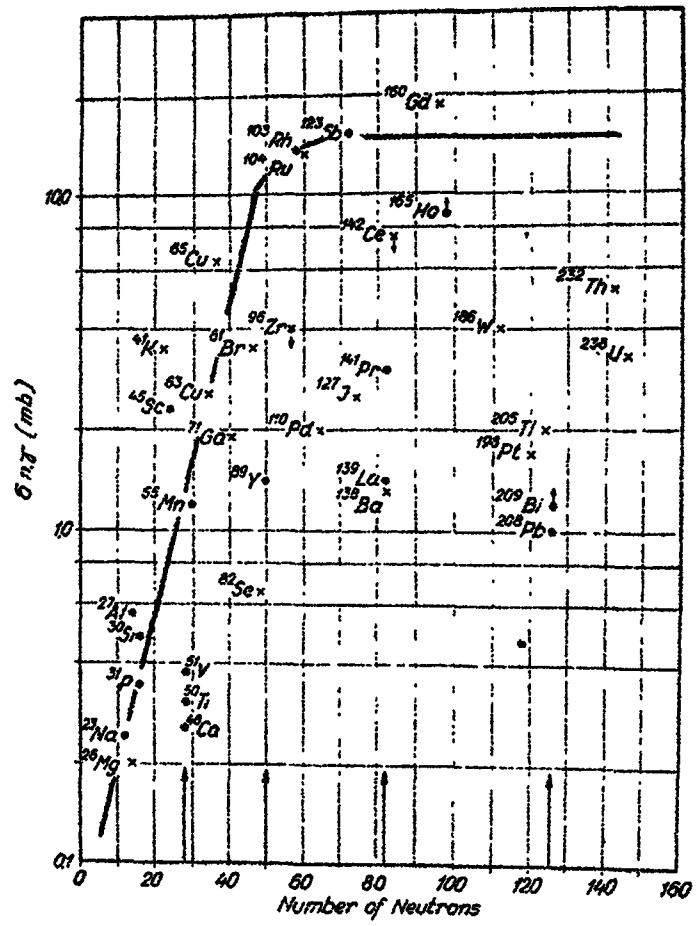

Fig.6. Radiative capture cross sections for 14 MeV neutrons.

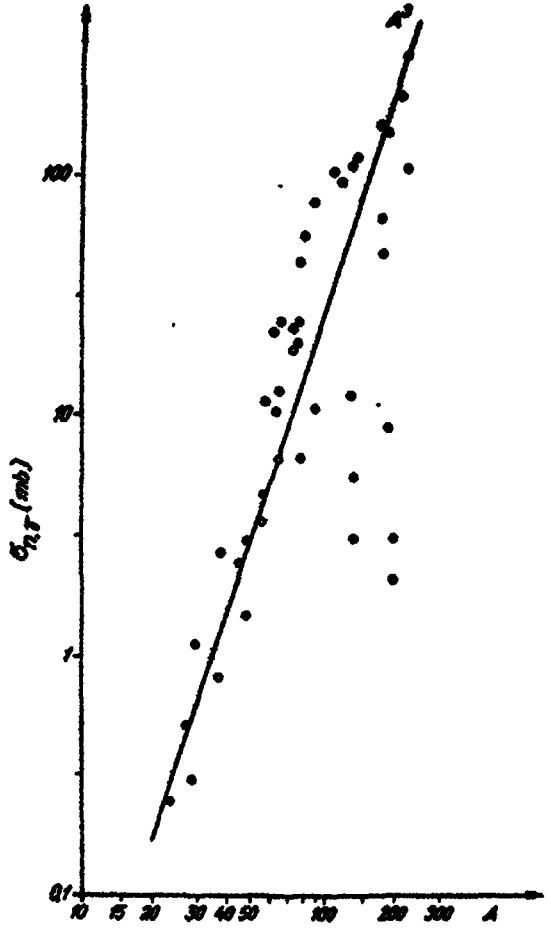

Fig.7. Radiative capture cross sections for 1 MeV neutrons as function of A.

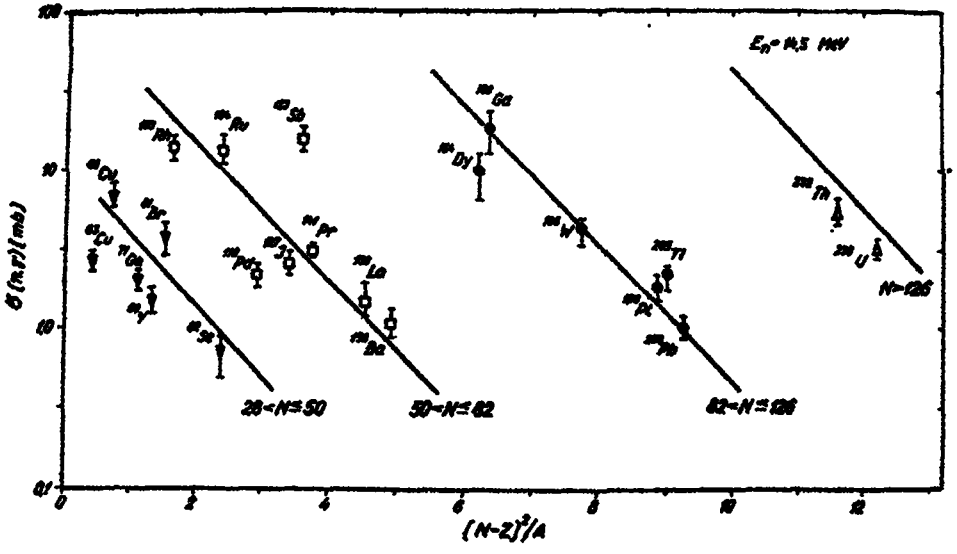

Fig.8. Experimental /n,γ/ cross sections plotted versus $(N-Z)^2/A$.

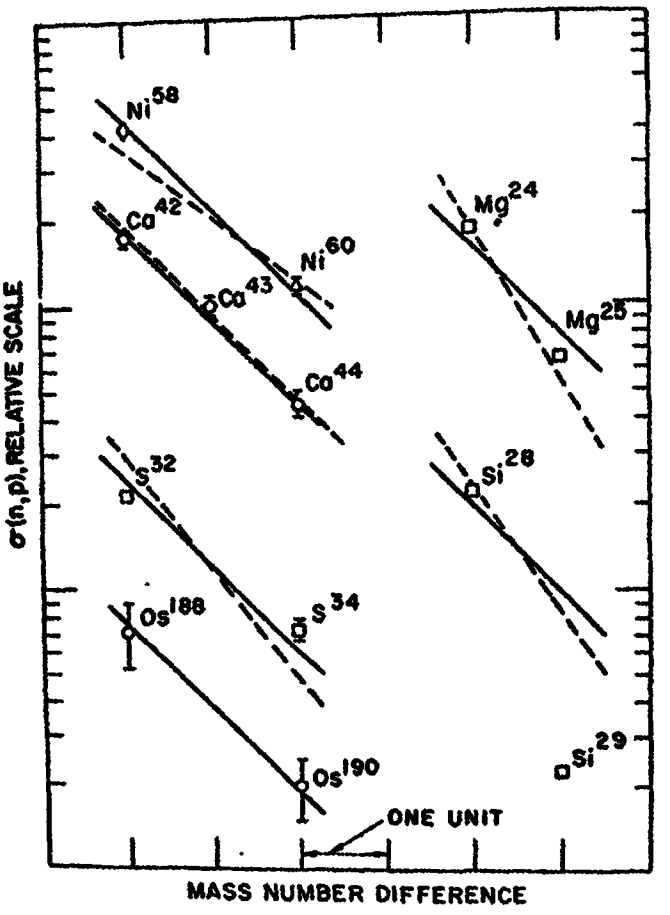

Fig. 9. Isotope effect in /n,p/ reactions. The solid lines are from Gardner and the dashed lines are from Levkovskii.

RECOMMENDED VALUES OF /n,2n/ AND /n,total/ CROSS SECTIONS

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The origin and the role of different errors in the measurements are discussed with particular interest concerning their possible elimination or correction. With a generalized averageing procedure most probable values were calculated for /n,total/ and /n,2n/ cross sections using experimental results from the literature. In the case of /n,2n/ cross sections further values were obtained by inter- and extrapolation using N-Z dependence previously observed; the cross sections for elements were also calculated by averageing over isotopic abundances.

While the spread in the total cross section data measured by different authors is approximately consistent with the given errors, the σ/n,2n/ values have gross desagreements ranging up to a factor of ten [1]. On the bases of several papers for /n,2n/ cross sections the different sources of errors are presented in Table I. The main part of the errors comes from the magnitude and angular

dependence of the flux and also from the uncertain decay schemes. The expected values of the systematic errors can be seen from the fact that the errors given by different authors amounts to 5-15 %, while the spread in the cross sections can reach an order of magnitude /Fig.1./.

It is useful to divide the errors into two groups:

1./ The errors of the measuring methods and instruments as well as evaluation procedures which may be called internal errors.

2./ Errors of the literature data used for evaluation /e.g. decay-scheme, half-life, standard cross sections, etc./ these may be called external errors.

The values of internal errors can be decreased by the authors using improved techniques for irradiation and activity measurements. On the other hand, the external errors can be corrected later by users, if the values and role of external data are given in the original article.

Valuable informations can be contained in papers giving a great number of cross section measurements even if the absolute values do not seem reliable. In some cases the unidirectional deviations can be corrected by an appropriate factor. As an example a set of measurements is given in Table II.

To obtain more reliable data a further possibility is the averageing of the available values. In this paper an averageing procedure is

given which was used to estimate the most probable values for the /n,2n/ and /n,total/ cross sections.

Let us suppose we have a number of cross section values $/x_i/$ and their errors $/s_i/$ measured by different authors. Following [12] a statistical model and an averageing procedure is given. The set of instruments /that is a number of parameters characterizing the measurement of the instruments/ used by different authors is considered as a statistical ensemble. The results obtained by each instrument is also considered as forming a statistical ensemble. One can say that the instruments constitute a macro-ensemble while the results of measurements by a given instrument constitute a micro-ensemble. So, there is only one macro-ensemble but there are as many micro-ensembles as instruments. The error associated with each instrument is split into two parts: systematic and statistical /random/ errors. The systematic error is the same for every element of a given micro-ensemble while the statistical error fluctuates in a random manner. In the macro-ensemble, however, the systematic error has a random distribution, i. e. the systematic errors of the micro-ensembles appear as a statistical error in the macro-ensemble. Further error which would be present in the macro--ensemble and would have a systematic character is excluded by assumption. All the distributions of errors are supposed to be Gaussian with zero means;

the statistical and systematic errors are taken to be independent. Using this model and the maximum likelihood principle the most probable value $\underline{m}$ can be calculated from the equations [12]

$$m = \frac{\sum_{i=1}^{N} \frac{x_i}{s_i^2 + y^2}}{\sum_{i=1}^{N} \frac{1}{s_i^2 + y^2}} \qquad /1/$$

and

$$\sum_{i=1}^{N} \frac{(x_i - m)^2}{(s_i^2 + y^2)^2} = \sum_{i=1}^{N} \frac{1}{s_i^2 + y^2} - \frac{\sum_{i=1}^{N} \left(\frac{1}{s_i^2 + y^2}\right)^2}{\sum_{i=1}^{N} \frac{1}{s_i^2 + y^2}} \qquad /2/$$

where $\underline{y^2}$ is the variance of the distribution of the systematic error and N is the number of measurements. The root mean square error Δm of $\underline{m}$ is

$$\Delta m = \frac{1}{\sqrt{\sum_{i=1}^{N} \frac{1}{s_i^2 + y^2}}} \qquad /3/$$

If Eqs. /1/ and /2/ have no solutions with $y^2 \geq 0$ then Eqs. /1/ and /3/ give the results with $y = 0$. One can see that when systematic errors are negligible compared with the statistical errors $/y^2/s_i^2 \to 0/$, the present method reduces to the well known expressions giving the weighted mean using reciprocal square of the errors:

$$m \rightarrow \frac{\sum_{i=1}^{N} \frac{x_i}{s_i^2}}{\sum_{i=1}^{N} \frac{1}{s_i^2}} \quad ; \quad \Delta m \rightarrow \frac{1}{\sqrt{\sum_{i=1}^{N} \frac{1}{s_i^2}}} \qquad /4/$$

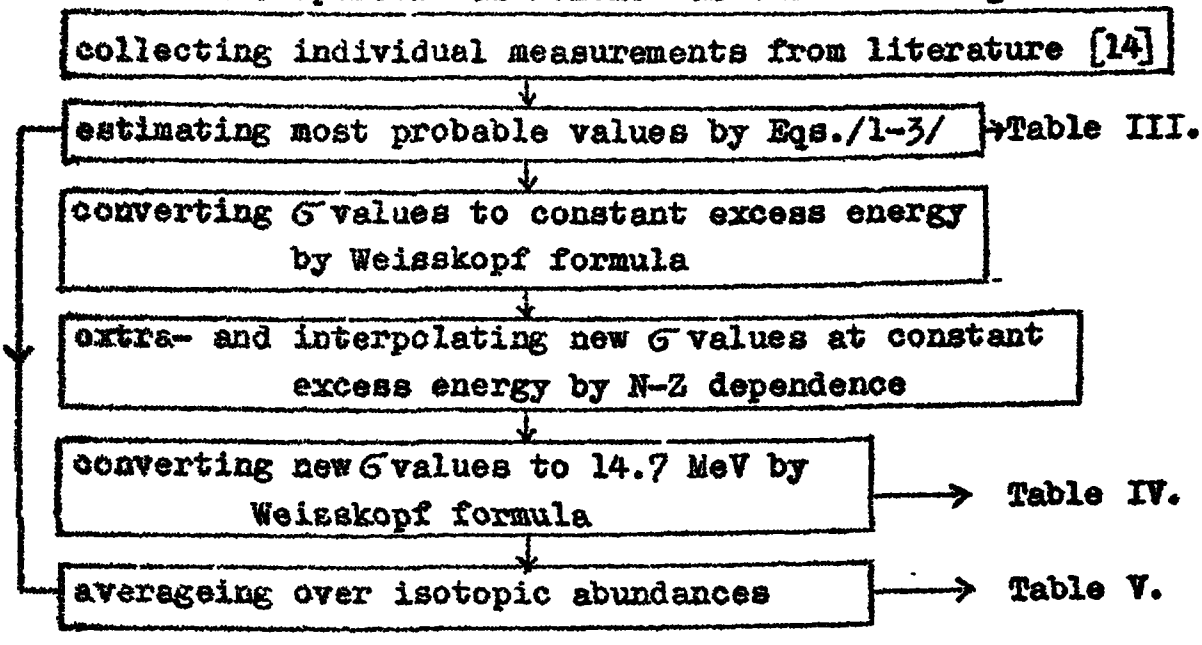
If statistical errors are negligible compared with the systematic errors $/s_i^2/y^2 \rightarrow 0/$ the present method reduces to one giving the simple arithmetic mean:

$$m \rightarrow \frac{\sum_{i=1}^{N} x_i}{N} \quad ; \quad \Delta m \rightarrow \sqrt{\frac{\sum_{i=1}^{N} (m - x_i)^2}{N(N-1)}} \qquad /5/$$

The most probable values for /n,2n/ cross sections at 14.7 MeV obtained by this averageing procedure are presented in Table III. For those nuclei where measurements are difficult to perform the cross sections were estimated using N-Z systematics [13] /see Table IV/.

So, having known the cross sections for isotopes the σ/n,2n/ values for elements /Table V./ were calculated by averageing over isotopic abundances.

The operational scheme was the following:



The averageing procedure applied to total cross sections in the energy internal 13-15 MeV was essentially the same as for /n,2n/ data. The total cross section values measured by different authors are approximately consistent with the given errors. Although there are some exceptions, on the average the inconsistency does not exceed 1 per cent. The grand means and their errors for various elements and isotopes are indicated in Table VI. For each atomic number the first line refers to the natural element.

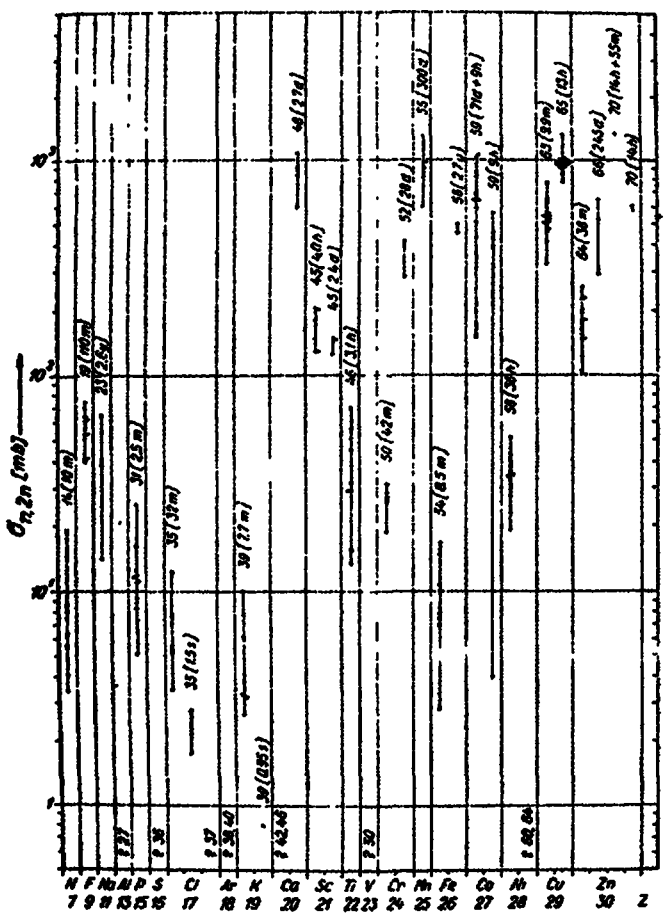


Fig.1. Activation cross section for /n,2n/ reactions around 14 MeV. The points for each nucleus show the experimental values obtained by various laboratories.

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Table I.

Sources of errors of cross sections in per cent

Quantity	References	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
FLUX	magnitude	5	3	4	4	6	8	7	4–8	–
	fluctuation	5	≤0.1	≪	0.1	–		–	–	–
	angular dependence	–	2.5	2.5	2.5	–	3	–	–	2.4
	sample geometry	–	2.5	3	1.7–3.8	–		0.5–1.5	1	1.4
	scattering by holder	–	≤0.5	0.5	0.5	–		–	–	0.5
	energy spread /KeV/	100	100–200	110–460	110–470	300	300	400–800	200–800	200
COUNTING	statistics		2.5–7.0	2	0.6–2.0	1		1	1	1
	efficiency	3		1.7	1.5–	3	2	1.4–	2	3
	self-absorption		1	≪	2.5	1–2		3	–	0.7
SAMPLE	weight	–	<0.1	≪	0.1	<0.1	–	–	0.5–	–
	chemical purity	–	<0.3	≪	0.3	–	–	–	2.0	–
DECAY	half-life	–	–	≪	–	–	1	–	–	–
	schemes	–	–	–	–	–	8	2.6–4	–	1.5
Measuring of time, dead time		negligible to others								
Total uncertainty		6–11	5–6	6–7	6	–	–	9.5	–	4.6
Reproducibility		–	≤2	–	≤0.7	–	–	–	–	≤2

Table II.

A set of cross sections measured by the same author compared with the average values. The $\sigma_{cor.} = 1.17\sigma$, where 1.17 is the average of the fourth column.

Nuclide	σ/mb/ ref. [11]	$\langle\sigma\rangle$/mb/ average	$\frac{\langle\sigma\rangle}{\sigma}$	σ_{cor}/mb/
^{14}N	5.4 ± 0.46	6.31 ± 0.9	1.17	6.3
^{19}F	38.9 ± 2.3	51.5 ± 4.8	1.32	45.5
^{45}Sc	130 ± 7.8	137 ± 8	1.05	152
^{46}Ti	13.3 ± 1.1	13.8 ± 0.9	1.04	15.6
^{63}Cu	409 ± 24.6	473 ± 22	1.16	478
^{64}Zn	105 ± 7	120 ± 5.3	1.14	123
^{69}Ga	755 ± 44	830 ± 50	1.13	860
^{79}Br	793 ± 48	847 ± 28	1.07	928
^{92}Mo	106 ± 7.5	137 ± 10	1.29	124
^{107}Ag	734 ± 44	838 ± 54	1.14	859
^{141}Pr	1240 ± 74	1663 ± 144	1.34	1450

Table III.

The most probable values of (n,2n) cross sections at 14.7 MeV.

Z	A	σ/mb/	$\Delta\sigma$/mb/	Z	A	σ/mb/	$\Delta\sigma$/mb/
7	14	7.67	0.7	35	81	1141	50
9	19	53.9	5.6	36	78	245	20
11	23	43.3	9	36	80	810	60
15	31	10.5	0.9	37	85	1438	93
17	35	9.2	0.7	37	87	1833	330
19	39	4.74	0.2	38	84	234	75
20	48	940	74	38	86	971	194
21	45	326	16	39	89	900	120
22	46	50.4	3.9	40	90	818	12
24	50	29.7	1.8	40	96	1456	80
24	52	352	66	42	92	194	12
25	55	896	44	42	100	2000	115
26	54	14.3	7	44	96	640	120
26	56	490	36	44	98	1169	91
27	59	883	87	44	104	1440	80
28	58	32.9	1.4	45	103	893	100
29	63	558	11	46	102	637	45
29	65	965.2	5.2	46	110	2050	470
30	64	190.7	15.3	47	107	1470	150
30	66	742.4	82	48	106	885	42
30	70	1307	130	48	108	865	100
31	69	1060	52	48	110	1221	150
31	71	1262	447	48	116	1566	40
32	70	663	10	49	113	1742	62
32	76	1311	49	49	115	1746	70
33	75	1111	34	50	112	1489	55
34	74	442	10	50	114	1550	250
34	76	937	70	50	124	1447	110
34	82	1400	150	51	121	1722	80
35	79	1069	39	51	123	1643	188

Table III. /cont./

52	120	1220	191	67	165	2170	300
52	122	1444	170	68	162	1870	300
52	128	1455	55	68	166	1965	115
53	127	1655	55	68	170	1895	133
54	124	1130	110	69	169	2000	115
54	126	1350	100	70	170	2080	110
54	128	1530	170	70	176	1810	130
54	134	1690	170	71	175	1940	150
54	136	1700	100	72	176	2220	115
55	133	1572	70	73	181	2220	370
56	130	1371	70	74	182	2200	100
56	132	1574	100	74	186	2290	230
58	136	1318	90	75	187	1568	112
58	140	1730	70	77	191	2100	140
58	142	1820	80	78	198	2300	230
59	141	1787	112	79	197	2122	180
60	142	1745	118	80	204	2234	123
60	148	1893	250	81	203	1704	170
60	150	1964	300	81	205	1990	280
62	144	1557	105	82	204	1833	180
62	154	1670	330	83	209	2214	100
64	154	1855	140	88	226	1600	200
64	160	1662	108	90	232	1280	80
66	160	2015	120	92	238	688	30

Table IV.
(n,2n) cross sections at 14.7 MeV obtained from N-Z systematics

Z	A	σ/mb/	Δσ/mb/	Z	A	σ/mb/	Δσ/mb/
20	44	512.3	42.7	46	105	1420.8	165.7
20	45	742.3	51.2	46	108	1759.9	202.6
20	43	554.3	80.2	47	109	1442.1	173.1
20	42	220.9	57.0	48	105	425.3	85.1
20	41	948.7	74.0	48	111	1256.4	174.8
22	46	39.4	3.9	48	112	1594.9	235.3
22	47	302.4	50.7	48	113	1557.9	229.9
22	48	322.2	42.2	48	114	1451.5	177.9
22	49	550.9	71.7	50	115	1554.2	113.7
22	50	553.1	53.1	50	116	1559.7	117.3
23	51	553.3	54.9	50	117	1527.3	115.7
24	55	808.0	141.0	50	118	1453.3	117.1
24	54	1115.7	151.3	50	119	1478.1	114.1
25	57	899.3	150.4	50	120	1454.7	115.8
25	52	1055.3	139.0	50	122	1458.2	115.5
26	50	438.1	58.5	52	122	1274.2	81.1
26	51	721.8	54.4	52	123	1290.3	79.9
26	52	890.5	59.1	52	124	1345.0	81.2
26	54	1093.2	90.0	52	125	1338.5	78.1
30	57	1023.0	79.0	52	126	1494.4	116.0
30	58	1158.6	65.7	52	130	1502.7	114.5
32	72	850.3	32.0	54	124	1423.3	114.3
32	73	1097.3	38.3	54	125	1475.5	114.9
32	74	1147.0	51.0	54	129	1525.3	113.1
34	77	1151.0	51.1	54	130	1573.0	115.2
34	78	1128.2	82.3	54	131	1554.9	112.2
34	80	1245.6	122.2	54	132	1527.1	115.0
36	82	724.9	77.5	56	132	1431.1	114.3
36	83	1120.9	125.4	56	134	1547.1	91.7
36	84	1200.0	151.3	56	135	1559.9	112.1
36	85	2012.0	166.2	56	136	1550.3	91.5
36	87	1472.3	124.9	56	137	1556.7	111.9
38	82	1411.2	107.0	56	138	1720.9	114.0
40	91	1151.4	48.9	57	139	1751.8	102.5
40	92	1253.2	49.3	58	135	1225.0	75.4
40	94	1340.1	51.3	58	138	1522.2	85.4
41	93	1052.0	56.1	60	143	1720.8	109.5
42	94	879.2	84.3	60	144	1797.1	112.3
42	95	1027.9	108.0	60	145	1774.5	109.2
42	96	1100.7	121.7	60	146	1843.5	111.7
42	97	1283.3	157.9	62	147	1891.6	153.8
42	98	1423.2	182.5	62	148	1825.3	157.1
44	98	940.8	54.9	62	149	1585.3	152.8
44	99	939.5	95.4	62	150	1543.5	153.5
44	100	958.0	99.1	62	152	1789.8	157.8
44	101	1110.1	107.1	63	151	1575.0	167.5
44	102	1253.2	72.4	63	153	1982.7	190.5
46	102	817.2	76.0	64	152	1792.4	224.0
46	104	945.9	118.4	64	155	1783.4	130.5
46	105	1275.4	141.7	64	156	1797.0	135.9

Table IV./cont./

Z	A	σ/mb/	Δσ/mb/
64	157	1725.6	130.3
64	158	1739.0	132.9
65	159	1874.6	144.2
65	160	1790.0	190.2
66	158	1907.6	189.5
66	161	2047.2	130.0
66	162	2157.5	132.8
65	163	2190.4	129.5
66	164	2349.3	154.7
68	162	2001.4	153.5
68	164	1996.2	132.2
68	167	1918.4	118.7
69	168	1927.9	120.5
70	169	1847.4	275.6
73	170	2047.3	110.1
70	171	1978.8	129.2
70	172	1958.7	131.3
70	175	1899.5	120.9
70	174	1898.3	150.2
72	174	2041.8	131.7
72	175	1990.5	97.4
72	177	1935.1	121.3
72	178	1976.2	141.2
72	179	2073.5	159.5
72	180	2234.3	151.2
74	180	2130.4	150.3
74	185	2178.3	159.4
74	184	2253.2	151.3
75	187	2230.1	151.9
75	184	2142.7	132.1
75	186	2142.1	132.7
75	187	2230.3	153.1
75	188	2141.4	152.2
75	189	2090.3	150.3
75	190	2142.8	151.5
76	192	2147.7	151.3
78	190	1990.2	103.1
78	192	2075.8	138.9
78	194	2152.7	152.3
78	195	2142.1	150.2
78	195	2203.9	151.2
75	185	2178.8	151.2
80	195	2060.3	154.3
80	198	2011.4	134.3
80	199	2021.7	150.3
80	200	2091.4	150.9
80	201	2038.2	157.9
80	202	2159.3	150.3
77	198	2139.5	151.3
82	205	1915.0	149.3
82	207	1929.8	156.2
82	209	1934.3	150.2

(n,2n) cross sections of elements at 14.7 MeV.

/Data for B, Li and Be were taken from ref. [15]/

Z		σ/mb/	$\Delta\sigma$/mb/	Z		σ/mb/	$\Delta\sigma$/mb/
1	H	26	3	50	Sn	1494	115
3	Li	60	10	51	Sb	1688	126
4	Be	500	100	52	Te	1495	90
7	N	7.67	0.7	53	J	1655	55
9	F	53.9	5.6	54	Xe	1597	120
11	Na	43.3	9	55	Cs	1572	70
15	P	10.5	0.9	56	Ba	1694	110
20	Ca	15	1.5	57	La	1732	103
21	Sc	326	16	58	Ce	1739	72
22	Ti	341	45	59	Pr	1787	112
23	V	565	55	60	Nd	1795	130
24	Cr	407	70	62	Sm	1668	196
25	Mn	896	44	63	Eu	1784	180
26	Fe	474	35	64	Gd	1741	127
27	Co	883	87	65	Tb	1875	144
28	Ni	183	15	66	Dy	2193	124
29	Cu	684	10	67	Ho	2170	300
30	Zn	565	48	68	Er	1933	120
31	Ga	1140	210	69	Tm	2000	115
32	Ge	982	40	70	Yb	1915	130
33	As	1111	34	71	Lu	1940	150
34	Se	1076	94	72	Hf	2090	144
35	Br	1105	45	73	Ta	2220	370
36	Kr	1320	145	74	W	2231	164
37	Rb	1548	160	75	Re	1791	130
38	Sr	1366	117	76	Os	2136	160
39	Y	900	120	77	Ir	2125	153
40	Zr	1038	33	78	Pt	2177	165
41	Nb	1082	86	79	Au	2122	180
42	Mo	1120	117	80	Hg	2100	160
44	Ru	1153	90	81	Tl	1906	250
45	Rh	893	100	82	Pb	1953	157
46	Pd	1491	200	83	Bi	2214	100
47	Ag	1456	160	90	Th	1280	80
48	Cd	1414	130	92	U	688	30
49	In	1746	70				

Table VI

The most probable values of /n,total/ cross sections between 13-15 MeV.

Z	A	σ/mb/	$\Delta\sigma$/mb/	Z	A	σ/mb/	$\Delta\sigma$/mb/
1	1.0081	0.5036	0.0049	30	65.4517	3.0012	0.0220
1	2.0000	0.5021	0.0149	30	64.0000	2.9650	0.0396
1	3.0000	0.9775	0.0110	30	66.0000	3.0710	0.0401
2	4.0000	1.0356	0.0102	30	67.0000	2.0900	0.0599
2	3.0000	1.1400	0.0714	30	68.0000	3.0510	0.0405
3	6.0225	1.4099	0.0230	30	70.0000	3.1130	0.0492
3	6.0000	1.4466	0.0100	31	69.7533	3.1824	0.0440
3	7.0000	1.4525	0.0206	32	72.5950	3.3400	0.0534
4	9.0000	1.4974	0.0120	33	75.0000	3.4054	0.1000
5	10.0057	1.5719	0.0142	34	78.9559	3.4736	0.0391
5	10.0000	1.4501	0.0149	35	78.9272	3.4920	0.0452
5	11.0000	1.4149	0.0204	35	80.9846	3.7767	0.0785
6	12.0139	1.5317	0.0087	38	87.7092	3.9800	0.0755
7	14.0036	1.5736	0.0175	39	89.9000	3.8545	0.0487
8	15.0043	1.5029	0.0184	40	91.3125	3.7441	0.2007
8	18.0000	1.4215	0.1848	41	93.0000	4.0053	0.0444
9	19.0000	1.7423	0.0170	42	95.9591	4.0128	0.0545
10	20.1795	1.7830	0.0225	42	96.0000	4.0400	0.1304
11	23.0000	1.7855	0.0150	43	99.0000	4.1954	0.0501
12	24.3232	1.7028	0.0091	45	103.9244	4.2798	0.0406
13	27.0000	1.7456	0.0135	47	107.9712	4.3237	0.0357
14	28.1057	1.8425	0.0228	47	107.0000	4.3400	0.0734
15	31.0000	1.8954	0.0214	47	108.0000	4.3800	0.0539
15	32.0914	1.9251	0.0125	48	112.5139	4.4455	0.0359
17	35.2449	2.0230	0.0191	48	113.0000	4.2800	0.1129
18	39.0950	2.1500	0.0563	48	109.0000	4.3500	0.1135
19	39.1570	2.1278	0.0310	48	110.0000	4.3400	0.0934
19	39.0000	2.2000	0.0729	48	111.0000	4.4400	0.0844
20	40.1125	2.1936	0.0105	48	112.0000	4.5500	0.0753
20	42.0000	2.2014	0.0425	48	113.0000	4.5000	0.0750
20	44.0000	2.1514	0.0574	48	114.0000	4.5400	0.0554
21	45.0000	2.1791	0.0533	48	115.0000	4.5500	0.0756
22	47.9227	2.3000	0.0159	49	114.9151	4.5305	0.0352
23	50.9975	2.3421	0.0311	50	118.8755	4.6058	0.0331
24	52.0555	2.4166	0.0222	50	112.0000	4.4100	0.0741
24	52.0000	2.4500	0.0645	50	115.0000	4.4300	0.1243
25	55.0000	2.5495	0.0310	50	117.0000	4.5400	0.0954
25	55.9101	2.5002	0.0106	50	118.0000	4.7500	0.1175
27	59.0000	2.5973	0.0292	50	119.0000	4.4600	0.1445
28	58.7715	2.6704	0.0213	50	120.0000	4.5500	0.0856
28	58.0000	2.7000	0.0350	50	122.0000	4.5900	0.0859
28	60.0000	2.7440	0.0354	50	124.0000	4.7100	0.1071
28	62.0000	2.7930	0.0380	51	121.9035	4.5647	0.0392
28	64.0000	2.8340	0.0303	51	121.0000	4.6500	0.0555
29	63.5454	2.8672	0.0173	51	123.0000	4.6800	0.0758

Table VI./cont./

Z	A	σ/mb/	Δσ/mb/
52	127.7154	4.0375	0.0545
52	122.9000	4.5500	0.0865
52	124.9000	4.5000	0.0960
52	125.9000	4.5900	0.0859
52	126.9000	4.7500	0.0375
52	128.9000	4.7500	0.0775
52	130.9000	4.9100	0.0681
53	127.9000	4.7927	0.0549
54	131.9154	5.0400	0.1320
56	137.4205	5.0998	0.0509
57	138.9091	4.9146	0.0750
58	140.9091	5.0007	0.0503
59	141.9000	4.9321	0.0574
60	144.9205	5.0140	0.0549
61	145.9000	5.5592	0.1425
62	150.4189	5.1755	0.0602
63	152.9434	5.1992	0.0809
64	157.9291	5.2511	0.0404
65	158.9000	5.2035	0.0752
66	162.5703	5.2550	0.0716
67	165.9000	5.2547	0.0505
68	167.9271	5.3544	0.0541
69	168.9000	5.3045	0.0711
70	173.9952	5.3350	0.0764
71	174.9233	5.3232	0.0774
72	178.5508	5.3447	0.0595
73	181.9000	5.2357	0.0473
74	183.9531	5.3365	0.0552
74	182.9000	5.4257	0.0774
74	185.9000	5.5191	0.0733
75	186.9577	5.1954	0.0621
76	190.9753	5.1545	0.0817
77	192.9291	5.2354	0.0825
78	194.9177	5.3701	0.0720
79	196.9000	5.3138	0.0452
80	200.9251	5.3473	0.0802
81	204.9092	5.4124	0.0491
82	207.9419	5.4078	0.0523
82	204.9000	5.4949	0.0934
82	205.9000	5.4154	0.0649
82	207.9000	5.3463	0.0847
82	208.9000	5.2950	0.0812
82	206.9000	5.2945	0.0657
83	209.9000	5.4224	0.0504
90	232.9000	5.5344	0.1295
92	237.9783	5.7493	0.0549
92	235.9000	5.7900	0.1279
94	239.9000	5.8500	0.1383

Interpretation of trends in total neutron cross sections

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Abstract

For medium and heavy nuclei, it is shown that the smooth dependence of the total neutron cross sections on mass number can be explained by a simple semi-classical picture, the so-called "nuclear Ramsauer effect" with reasonable values of the real optical potential depth and surface thickness. At 14 MeV neutron energy data seem to suggest a strong surface absorption. Extending the investigation to different energies, it was found that the above picture can be applied to the interpretation of the total cross sections for E > 10 MeV only, though a simple formula of practical interest holds also for lower energies. Some refinement can be attained using a corrected form of the blanck nucleus formula.

For light nuclei, a correlation between the nuclear radius parameter r_0, and the average binding energy per nucleon E/A, was found. Results of Hartree-Fock calculations for light nuclei also show this correlation.

The total neutron cross sections for $A \geq 27$ and $0.5 \leq E_n \leq 42$ MeV can be described by a simple empirical expression [1,2] of the form:

$$\sigma_T = 2\pi(R+\lambda)^2\left[a - p\cos\left(qA^{\frac{1}{3}} - \pi\right)\right] \qquad (1)$$

where $R = r_0 A^{1/3}$, $\lambda = 1.22\ \frac{A+1}{A}$ f. The values of a, p, q and π parameters for different energies are given in Figs. 1-3. As an illustration Figs. 4,5,6 show the σ_T/σ_{BN} data and the calculated values /dashed line/ as a function of $A^{1/3}$ for E_n = 5, 14 and 24.8 MeV.

The sinusoidal form can be explained using the general formulae for the cross sections

$$\sigma_S = \pi\lambda^2 \sum_\ell (2\ell+1)\left|1-\eta_\ell\right|^2 \qquad (2a)$$

$$\sigma_R = \pi\lambda^2 \sum_\ell (2\ell+1)\left(1-|\eta_\ell|^2\right) \qquad (2b)$$

$$\sigma_T = 2\pi\lambda^2 \sum_\ell (2\ell+1)(1-\mathrm{Re}\,\eta_\ell) \qquad (2c)$$

where $\eta_\ell = \exp(i\Delta_\ell)$, Δ_ℓ being the phase shift between the wave traversing the nucleus and that going around it.

Assuming $\eta_\ell = \eta = \rho\exp(i\delta)$ for

$\ell \leq \ell_{max} = R/\lambda$

and $\eta_\ell = 1$ for $\ell > \ell_{max}$ where

$\rho = \exp(-\mathrm{Im}\,\Delta)$ and $\delta = \mathrm{Re}\,\Delta$, we have

$$\sigma_S = \pi(R+\lambda)^2\left(1+\rho^2-2\rho\cos\delta\right) \qquad (3a)$$

$$\sigma_R = \pi (R+\lambda)^2 (1 - \rho^2) \qquad 3b$$

$$\sigma_T = 2\pi (R+\lambda)^2 (1 - \rho \cos\delta) \qquad 3c$$

If $\rho = 0$, $\sigma_S = \sigma_R$ and for σ_T we get the "black nucleus" formula. For $\rho \neq 0$ an oscillating term appears both in the scattering and total cross sections, and $\sigma_S \neq \sigma_R$
It should be noted, that expressions similar to eqs. (3a) and (3b) have been used in ref. [3] to describe the scattering of 90 MeV neutrons. According to the measurements of McGregor et al. [4] the nonelastic cross sections are close to the geometric values, and so the oscillation of total cross section is caused only by the elastic scattering process.

The phase shift δ can be determined from the nuclear Ramsauer effect, that has been successfully used for the location of maxima and minima in neutron total cross sections [5], and also for calculation the difference in the total cross section due to nuclear orientation [6]. The phase shift caused by a sphere of radius R and index of refraction n is [5]

$$\delta = \bar{C}(n-1)/\lambda = c\, 2r_0 A^{\frac{1}{3}}(n-1)/\lambda = \text{const.}\, A^{\frac{1}{3}} \qquad (4)$$

where the average chord length C is proportional to $A^{1/3}$. The good fit of the calculated curve to the experimental data suggests that n is independent

of A. For example at 14 MeV, equating the const. in eq. (4) to the frequency constant q of the empirical formula (1), we get $n = 2.015$ for the index of refraction and an optical potential depth $U = 42.8$ MeV.

The phase constant r in the empirical formula (1) can also be explained. Assuming that a surface thickness t exists in which the index of refraction changes, we have for the phase shift

$$\delta^* = (\bar{c} - 2t)(n-1)/\lambda + 2t(\bar{n}-1)/\lambda = \\ = \delta - 2t(n-\bar{n})/\lambda \qquad (5)$$

where n is the average value of the index of refraction within t. It can be seen that a new term appears in the phase shift and this is independent of the mass number. Supposing that the potential decreases linearly in the surface region, the value of t can be calculated from the observed phase constant r. Performing this, a value of $t = 1.6$ fm was found for 14 MeV.

It should be noted that a simple volume absorption would result in an exponentially damped oscillation of σ_T/σ_{BN} in the function of $A^{1/3}$. The nearly constant amplitude of oscillations, however, suggests that absorption on the surface is much stronger than in the volume. Assuming the same surface thickness $t = 1.6$ fm for absorption as for the phase shift, from the 14 MeV data we have $W_V \approx 2$ MeV and $W_S \approx 40$ MeV for the volume and surface imaginary potential, respectively.

The value of the parameter a is about unity for neutron energies higher than 10 MeV, while for E < 10 MeV it drops with decreasing energy. This can be seen in Fig.1.; here $E^{1/2}$ is used as independent variable, because this seems to be the appropriate quantity in the nuclear Ramsauer picture.

No similar behaviour can be found in the amplitude of the oscillation, p /see Fig.1./. There seems to be only a slight, approximately linear decrease with increasing $E^{1/2}$.

The values of the frequency parameter q are plotted in Fig.2. A monotonic decrease with increasing $E^{1/2}$ can be explained easily, using the nuclear Ramsauer picture, because - as shown in ref. [1] - this is essentially proportional to

$$q \propto \frac{n-1}{\lambda} \propto \sqrt{E+U} - \sqrt{E} \qquad (6)$$

A more detailed investigation of the parameters shows that the nuclear Ramsauer effect can be applied to the interpretation of the total cross sections for $E \geq 10$ MeV only.

It should be noted however, that using parameters as shown in Figs. 1-3, (1) describes the cross sections also for lower energies. This is extremely useful from the practical point of view, because it gives a possibility to describe the gross structure of the $\sigma_T(A,E)$ surface - found by Barschall et al. ref. [7] - by a

simple formula in a considerable energy and mass number interval. In addition to the practical importance, the sinusoidal form of the σ_T/σ_{BN} plots for energies lower then 10 MeV, leaves open the possibility of further improvements on this simple model.

One such improvement may be the use of a better approximation for the black-nucleus formula. Supposing that only those partial neutron waves interact with the nucleus, for that the kinetic energy is not lower than the centrifugal potential barrier, we have:

$$\sqrt{l_{max}(l_{max}+1)} = R/\lambda \qquad (7)$$

Using this, the corrected black-nucleus formula is

$$\sigma'_{BN} = 2\pi\left(\sqrt{R^2+\left(\frac{\lambda}{2}\right)^2} + \frac{\lambda}{2}\right)^2 \qquad (8)$$

If $R^2 \gg (\lambda/2)^2$ we have

$$\sigma'_{BN} = 2\pi\left(R+\frac{\lambda}{2}\right)^2 . \qquad (9)$$

i.e. smaller than that used generally. Using (8) as σ_{BN} we get lower black-nucleus values, i.e. higher σ_T/σ_{BN} ratios, and so the parameter a increases especially for low energies. Crosses in Fig.1. stand for these new values.

In the region of light nuclei there are considerable deviations from the "black nucleus"

formula. In order to perform a systematic investigation, total cross sections were measured under the same experimental conditions [8]. Measured total cross sections, together with data from other sources, were divided by the "black nucleus" formula using $r_0 = 1.4$ f and $\lambda = 1.2$ f and are plotted in Fig.7. as a function of Z /filled circles/.

As can be seen in the figure, the reduced cross sections show a decreasing tendency for increasing Z, with definite deviations for some nuclei. This structure can be caused by a variation either in r_0 or in the "opacity" of the nuclei. The question is answered by plotting the normalized electric charge radii [9] $r_{0,el}/r_{0,el}(Na)$ for the light nuclei /crosses in Fig.7./. One can conclude that the deviations observed in total neutron cross sections are caused by r_0, i.e. the average distance between nucleons in light nuclei varies significantly.

These variations in r_0 should be connected with other average properties of nuclei, e.g. to the binding energy per nucleon, $\mathcal{E}$; an increase in r_0 should cause a decrease in $\mathcal{E}$. To confirm this assumption, the values of $1/\bar{\mathcal{E}}$ were also plotted [10] /circles in Fig.7./. In calculating the average $\bar{\mathcal{E}}$ for an element, the isotopic $\mathcal{E}$ values were weighted with the isotopic abundances. The insert part of Fig. 7 shows the values of $(r_0 \bar{\mathcal{E}})/(r_0 \bar{\mathcal{E}})_{Na}$ against Z, verifying that the relation $r_0 \propto 1/\mathcal{E}$ is approximately valid. $(r_0 \cdot \mathcal{E})_{Na} = 11.35$ MeV.fm from

σ_T measurements, and $(r_{0,el.}\xi)_{Na} = 10.87$ MeV.fm from electric charge radii./

The two- and three-nucleon systems, like ^2H, ^3H and ^3He are exceptions. The relation r_0 (fm)= $= 11/\xi$ (MeV) obtained above, gives an exceptionally high r_0 value, although the correlation between r_0 and ξ exists for these nuclei, too.
It is interesting to note that r_0 and $\bar{\xi}$ values deduced from the results of Hartree-Fock calculations also show this correlation. Results from density dependent effective interactions [11] and the B1 force of Brink-Boeker [12] are presented in Fig.8. As it can be seen, the $r_0 . \bar{\xi}$ product is approximately constant for both calculations, but their absolute values differ significantly. Arrows show results for identical nuclei, i.e. the strength of forces can be checked by this correlation.

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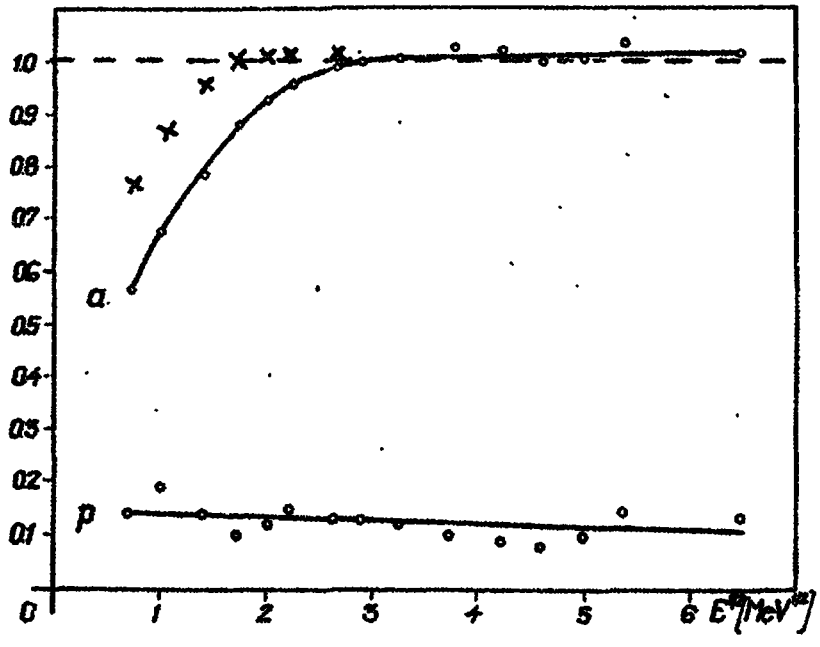
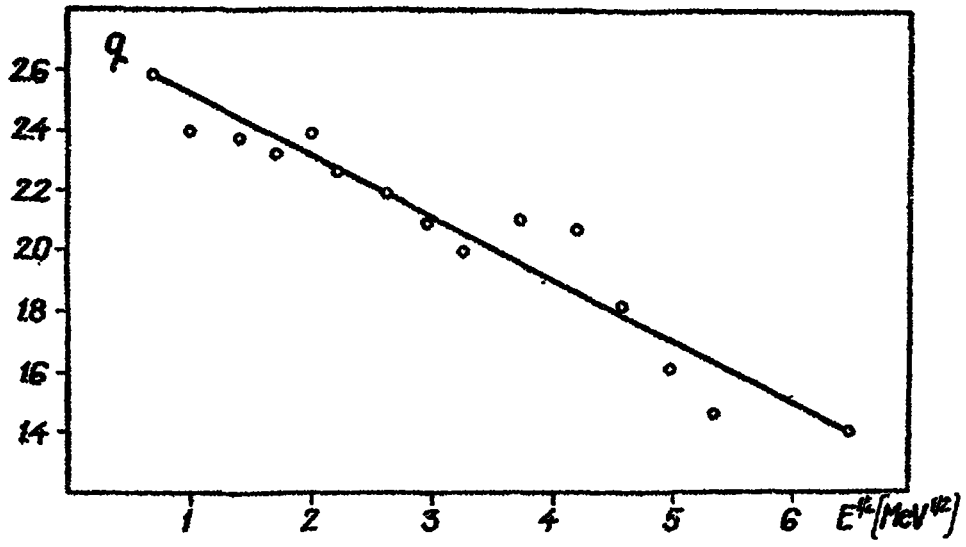


Fig.1. Values of parameters a and p as a function of $E^{1/2}$; crosses: a-values using the corrected black nucleus formula.



ig.2. Values of the parameter q as a function of $E^{1/2}$.

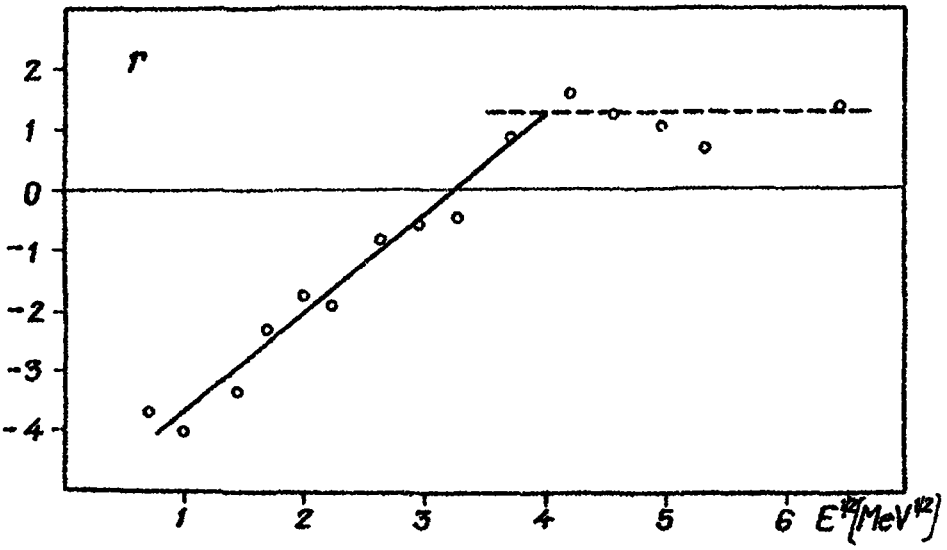


Fig.3. Values of the parameter r as a function of $E^{1/2}$

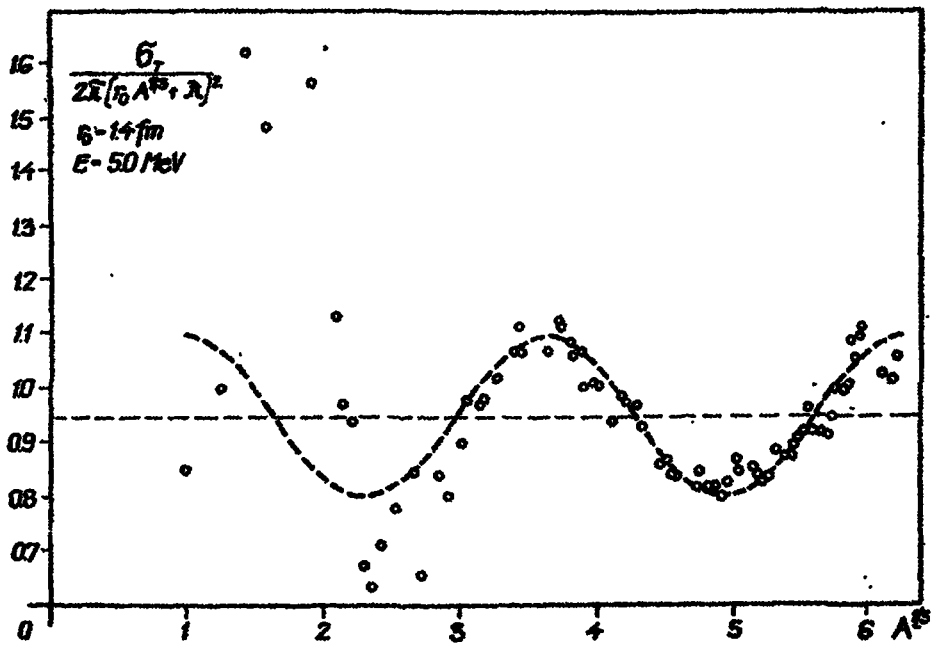

$\frac{\sigma_T}{2\pi(r_0 A^{1/3}+\lambda)^2}$
$r_0 = 1.4$ fm
$E = 50$ MeV
A^{1/3}

Fig. 4.

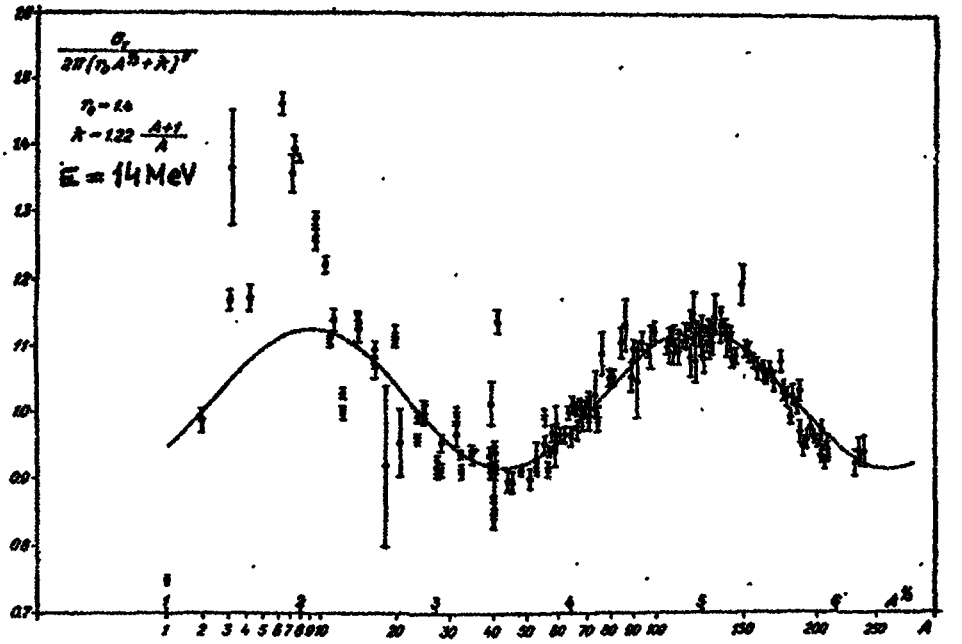

$\frac{\sigma_T}{2\pi(r_0 A^{1/3}+\lambda)^2}$
$r_0 = 1.4$
$\lambda = 1.22\frac{A+1}{A}$
$E = 14$ MeV
A^{1/3}
A

Fig. 5.

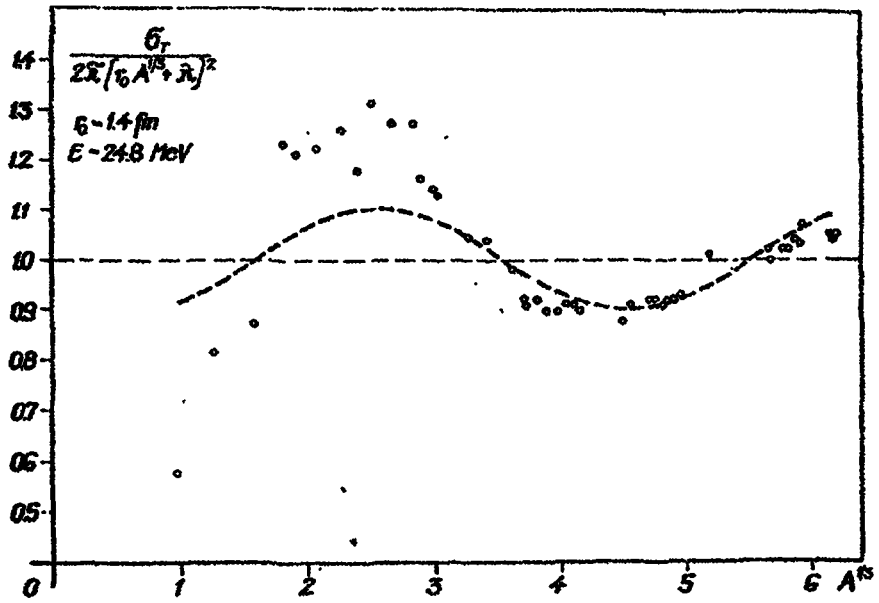


Fig. 4.,5.,6. Experimental total neutron cross sections divided by the black-nucleus value as a function of $A^{1/3}$. Dashed line: best-fit curves $A \geq 27$ of the form eq. (1) .

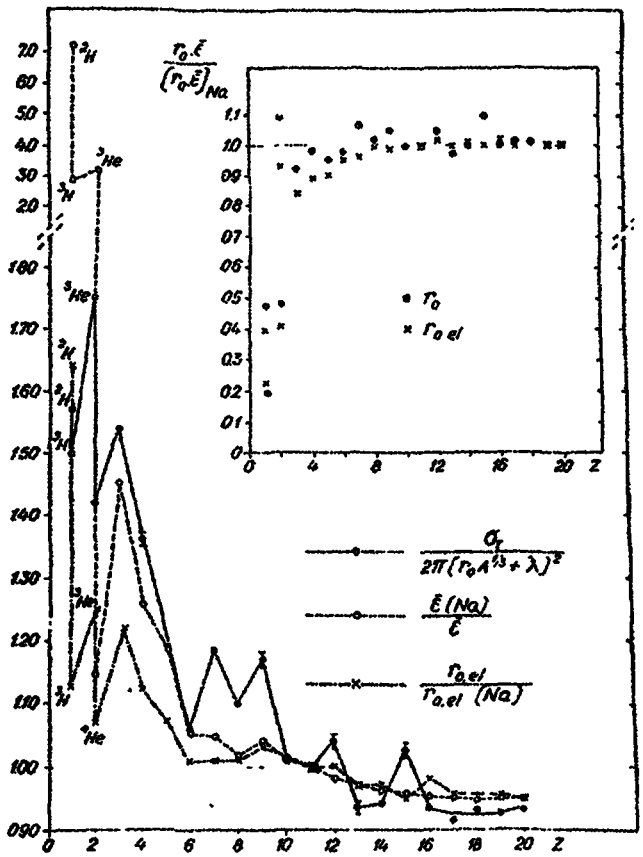


Fig.7. Reduced total neutron cross sections /filled circles/, electric charge radii /crosses/ and reciprocals of average binding energies per nucleon /open circles/, normalized to sodium, versus proton number. The insert shows the values of $(r_0.\bar{\varepsilon})/(r_0.\bar{\varepsilon})_{Na}$.

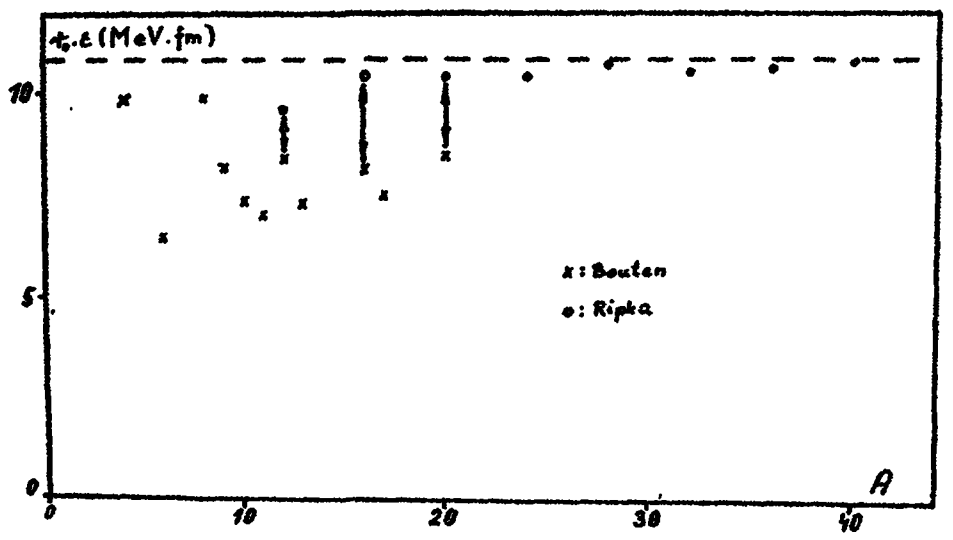


Fig.8. $\hbar_0.\bar{\varepsilon}$ values from H-F calculations as a function of mass number. Open circles: density dependent effective interactions [11] ; crosses: B1 force of Brink-Boeker [12]; dashed line: experimental value.

Establishment of Computer Libraries of Evaluated Data and Associated Computer Programs

by

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Abstract

The preferable features of a computerized library for evaluated data are reviewed. The importance of checking and editing codes operating on the data library is discussed with examples given of their use. Format problems and their influence on the exchange of evaluated data libraries are also appraised.

Introduction

In order for a computerized library to be considered reliable and therefore enjoy widespread use the following conditions should be satisfied.

1. The format should be adequate for storage of all pertinent information and flexible enough to be extended to all new types of information.
2. The format should be compatible for use on a wide variety of computers to allow exchange of information.
3. The format should be relatively efficient and well documented in order for data to be processed without confusion.
4. For important reactions the library should contain suitably referenced data files that are consistent with the best differential and integral data available.
5. Checking codes should be available to test the internal consistency and the physics content of the files to not only assist in the

initial preparation of error free data sets but to ascertain whether errors are inadvertently introduced at a future time (quality control).

6. A good communication link should be established between measurer, evaluator, and user to ensure that new data and data testing experience are factored into revisions to the evaluated data library.

Formats, Editing and User Programs

The formats should be adaptable to computer processing. Useful features are separation of text from numerical information, indices to indicate length of tables to be processed, computer independent file indicators, etc. The formats should be flexible enough to allow the evaluator sufficient choice for the entry of data but not so flexible as to require a large programming effort to accomodate an excessive number of format possibilities in application studies. The construction of new formats should be based on experience gained through the use of older formats.

Editing of the data files into various output forms should be provided. Listings and graphs should be furnished which require no knowledge of the format for comprehension of the data, i.e. internal numerical equivalents of reactions and units are translated into readable forms. The computation of additional basic quantities should be possible such as cross section averages over specific ranges of a Maxwellian, 1/E, and fission spectrum; neutron age in pure materials; alpha, if only the capture and fission cross section are provided; etc. It should also be possible to convert data to various output forms, as in the case of converting from resonance parameters to Doppler broadened tables, and the application of various resolution functions to the evaluated data for comparison with the measurements.

Programs should be written that directly couple the library format to the input stage of major application codes to facilitate the processing of data.

A universal preprocessing code is probably not possible because of the often different library requirements of diffusion theory, transport theory, and Monte Carlo codes.

Practical Problems of Representing Evaluated Data

Data representations should have one and only one possible interpretation. The documentation describing the library format should explain factors affecting both the programming and physics use of the format and sufficient examples should be included in the documentation to assist both those who are entering data and those who are using data.

The data representation should be fairly compact and should use such techniques as resonance parameters instead of large tables of cross sections at many temperatures and Legendre coefficients instead of tabulated angular distributions. It is recognized that tabular representations rather than resonance parameters may result in a net savings of computer time and may be more convenient to use. Similarly, Legendre polynomial representation may not be appreciably more compact than tabulated angular distributions and the latter may be appreciably more convenient in some applications, e.g. Monte Carlo techniques. Representations should also be compatible with current usage of data in application programs. For example, even though Bessel functions can represent angular distributions reasonably, only Legendre coefficients are widely used in reactor physics codes. Wherever practical, representations that are mathematically convenient and also relate to physical theories should be used, as in the case of resonance parameters in the resonance region and nuclear temperatures in secondary energy distributions, but in no case should good representation of the physics be subordinated to mathematical convenience.

Data sets must be both internally and externally consistent.

The individual data sets should be properly normalized so that differential cross sections and spectra are compatible with integral values, partial cross sections add up to the total cross section, fission yields sum to the proper value, etc. The cross section should be continuous and single valued at boundaries where the representation changes such as between an energy region described by resonance parameters and a region described by tabulated values.

The cross sections for individual materials must be consistent with pertinent information for other materials. Cross sections for separated isotopes must agree with data available for the natural element. The cross sections of individual data sets should not only be consistent with absolute measurements for that material, but with measurements of cross section ratios between different materials. Wherever feasible, widely accepted compilations of nuclear masses isotopic abundances, decay constants, 2200 M/S cross sections, etc., should be used as source material for the evaluated data library.

Adequate checking codes are required both to assist in the initial preparation of data sets and to determine whether the data sets are accidentally changed in the future. The data sets should be checked for numerical consistency and physical content. Format checks and numerical consistency checks such as for deviant points and agreement between indices and length of files are necessary for reliable processing of the data by computer codes. The performance of physics checks on the data will not only assist the computer processing of the library but will provide information about the quality of the data sets. Examples of physics checks are the comparison of reaction threshold energies given in the file with calculated thresholds from a stored mass table and the comparison of the 0^{o} differential elastic scattering cross section with Wick's limit. In addition, the calculation of various quantities, such as resonance integrals from the microscopic data, for comparison with

integral measurements will help determine with what confidence the data set can be used.

Technical Problems Connected With the Exchange of Evaluated Data Libraries-Conversion from One Format to Another

Experience with the exchange of experimental neutron data has shown that use of a common format facilitates the entry of data into each center library and the answering of requests for information. However, several formats are extensively used to store evaluated data. These libraries have some important differences in format and content. Each format is probably uniquely coupled to a set of major processing codes. These factors inhibit the ready adoption of new and different formats.

The conversion of one format to another is a major programming effort and can be made increasingly difficult by lack of proper format documentation. Technical decisions must be made when a one to one correspondence does not exist between library formats as occurs in the representation of secondary energy distributions in several major formats. In addition, the nonuniform use of representations may weaken the incentive for translating data from one format to another such as the use of tabulated data in the resonance region in one format where resonance parameters are favored in the other format.

The exchange of evaluated data will depend therefore on the ability to define acceptable formats for the exchange of data, the availability of programming effort for necessary format conversions, and the degree to which tested data sets exist in the various libraries to stimulate the exchange of evaluated data.

Technical Comments and remarks about ENDF/B, KEDAK and UKNDL

by

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Abstract

Some of the technical problems encountered in automatically handling evaluated data libraries are discussed. The paper also presents recommendations for allieviating some of these difficulties.

1. Redundant information - Sometimes redundant information is given in the file. In KEDAK, for example nuclear data in the resonance region is represented by resonance parameters as well as by tables of the cross sections as a function of energy. The number of fission neutrons is represented by a lengthy table as well as by a polynomial representation and so on. Since an evaluated library should give its user only a "single best" value, the library itself should contain some sort of a priority control number for such redundant files, so as to enable an automatic code to ignore the redundant information and chose one preferred set of data.

2. Assessment of errors of evaluated data - If errors or ranges of uncertainty for evaluated data are assessed they should be documented on the library tape itself. This should be done in an alphanumeric file (such as file 1 in ENDF/B). These estimated errors should also be included in the beginning of each subfile or data table so as to enable an automatic code to use it. This can be done by a table such as ERR(I), EL(I), EH(I), ERR(2), EL(2), EH(2),... where ERR(I) is estimated error in the I-th energy range and EL(I), EH(I) are lower and upper limits of that range.

3. User programmes - User programmes for correcting, updating, plotting the data of any cross section of any isotope at any requested energy range and the associated programmes for the production of multigroup cross sections should form an integral part of the "package" library. Some of these user programmes require huge computers (65 K words) with many tapes and long running times. This reduces the possible use of these programmes in centers having moderate computer facilities.

The IAEA should gather information about the existence of economic and efficient service programmes that could be used by centers with moderate computer facilities.

4. Head cards for subfiles.- In writing an automatic code that processes a library tape an extreme care should be taken not to lose the information written on the first card of the subfile. This is somewhat difficult because the code does not "know" which subfile is started until it has already read the first card. The simplest way to avoid this difficulty is to insert a head card that contains no information save that of the subfile identification numbers. These numbers should pass control to the appropriate section of the automatic code, and processing of the subfile is continued. This will also make the library much more flexible because the orderof the subfiles will lose its importance, and additional subfiles could be added at the end of the existing file.

5. "Standard blocks" at the beginning of library tapes - A library tape written in one country might be rejected as "faulty" by a tape reader if the synchronization between the writing tape recorder and the reading tape recorder is poor. In order to establish the synchronization between the tape recorders, some standard blocks (for instance an accordance with IBM technical specifications) should be written on the tape just before copying the library. These blocks will serve as a standard in case of difficulty.

6. Order of subfiles - Conversion from one format to another will be relatively easy if the order of the subfiles will be the same in all libraries. If this could not be agreed upon because of the changes needed in some of the existing libraries, at least comment 4) on head cards for subfiles should be adopted.

7. Resolved and unresolved resonances - The fitting of resonances data to a single level Breit-Wigner formalism should be given in all cases. If better fits to the Adler-Adler or Reich-Moore formalisms are available, they should be given in "redundant" information. Estimated errors, if possible, should also be included.

REMARKS ABOUT UKNDL, ENDF/B-II AND KEDAK LIBRARIES

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ABSTRACT

Some notes on the nuclear data collections merging up from a daily familiarity with the relate data files are listed.

This writing would plead assiduous customer's cause in daily using the computer libraries, roaming to-day about the world, concerning evaluated nuclear data. UKNDL, ENDF/B-II and KEDAK are generous mines of information, which many people work around both in trying to improve and in using them properly and easily. Their efficacy is well known, but we wish to list some small disadvantages occurred to a continuous user with a view to both advertising the people in order to avoid surprises and obtaining help from he who has already got over the handicap. The topics are shared among the three above mentioned nuclear data libraries (which will be thus abbreviated: U=UKNDL, E=ENDF/B-II, K=KEDAK) and are grouped under three subjects.

1. FORMATS, EDITING AND USER PROGRAMMES

1.1. Formats

U. This format is unchanged from birth, which is very advantageous from the point of view of the computer programmes written or planned to accept this file; on the other hand the amount of new data requires new sections to be added to the existing ones in order to allow, for example, more inelastic levels and the resonance parameters. In addition, it seems not to be negligible the missing, within each DFN, of an item unequivocally establishing whether a material is an isotope or an element or a mixture.

E. This collection would spare more computer time if an index of contents were included at the top of each tape.

K. Retrieving a material from a tape is difficult and time wasting. Several sequential functional values might be avoided when zeroes.

1.2. Editing and user programmes

U. NDF PRINT, IDA and CHECK seem to be still today up-to-date enough, while other codes, such as TEMPO, need some improvements.

E. The equipment is various and abounding in codes, but not all programmes run the first time we put them into our computer. In addition the last release of some codes is not completely checked.

K. No attached codes are released for this nuclear data file.

2. PRACTICAL PROBLEMS OF REPRESENTATION OF EVALUATED DATA

In general, as far as the Doppler broadening problem is concerned, a good improvement should be that of giving tabulated cross section curves together with the resonance parameters; in addition the averaged parameters in the unresolved region must exactly reproduce the tabulated cross section.

U. a) No information is given in the nuclear data file concerning the sources and the methods adopted for the evaluation.
b) More significant figures would be necessary to represent the energies, mainly in the resolved resonance range.
c) Legendre coefficients should be very appreciated to describe angular distributions if cross section positive values were assured over the whole angular range.

E. No criticism from this point of view.

K. a) See 2.U.a and 2.U.c.
b) Angular distribution normalization to unity would conform to the general rule adopted by several computer programmes.
c) Secondary energy distribution laws, although announced in the introductory report, are not given in this release.
d) An accurate description of the interpolation criteria is missing.
e) The label field of the card image format (cols. 73-80) is not sufficiently descriptive of either the nuclide or the reaction.

3. TECHNICAL PROBLEMS CONNECTED WITH THE EXCHANGE OF EVALUATED DATA LIBRARIES-CONVERSION FROM ONE FORMAT TO ANOTHER

In general it would be very useful to adopt a unique energy unit for the three sources in order to simplify the comparison and the translation from one format into another.

The problem of exchanging data from one area to another where a different format is in use, has been met with effort by several people: two years ago, owing to our laboratory's needs, we also were entrusted with such an enterprise and two programmes were the result of the work: UTOE for UKNDL into ENDF/B and KTOE for KEDAK into ENDF/B translations. Being interested in cross sections and angular distributions only, we met the problem of translating the secondary energy distribution laws (U into E only) in a very rough and provisional way; but we had the opportunity to find that point to be the big problem of a translation because of different law numbers, different law structure, different energy units, different array sizes. To-day codes such as UKE, LATEX, LUTE seem to have settled the question in the U into E sense, at least, and viceversa. Attempts concerning the K into E direction are being developed. Finally, our mind is that the best way to solve the problem sparing computer time is planning production programmes accepting the three sources (and others which are borning) directly as input.

ФОРМАТ БИБЛИОТЕКИ РЕКОМЕНДОВАННЫХ ЯДЕРНЫХ ДАННЫХ ДЛЯ РАСЧЕТА РЕАКТОРОВ (состояние на март 1971 г.)

В.Е.Колесов, М.Н.Николаев

А Н Н О Т А Ц И Я

Описывается формат хранения информации в Библиотеке рекомендованных ядерных данных ФЭИ. Его важная особенность заключается во введении специальной классификации данных по типу представления. Это позволяет реализовать различные способы задания данных для одного и того же типа реакции и, тем самым, существенно расширить возможности системы хранения рекомендованных ядерных данных.

В библиотеке предусмотрено хранение нейтронных данных в подгрупповом представлении с различным числом подгрупп нейтронов. Подгрупповое представление является удобным способом задания данных в области неразрешенных резонансов.

Излагаемый здесь формат хранения данных является дальнейшим развитием формата, описанного в докладе, представленном на Советско-бельгийско-голландский семинар по некоторым вопросам физики быстрых реакторов (Мелекесс, февраль 1970 г.)

В настоящее время основная масса расчетов ядерных реакторов осуществляется с помощью многогрупповых методов и, вероятнее всего, такое положение сохранится ещё достаточно долго. Ещё недавно подготовка систем многогрупповых констант требовала настолько значительных затрат труда и времени, что практически возможным было использование систем констант с фиксированным разбиением области энергий нейтронов в соответствии с типом рассчитываемых реакторов. Вместе с тем такому подходу присущ ряд очевидных недостатков, вытекающих как из неуниверсального характера получающихся таким образом систем констант, так и технической сложности внесения в них изменений.

Развитие вычислительной техники позволяет в значительной степени автоматизировать процесс переработки набора рекомендованных ядерных данных с точечным представлением величин в групповые константы с произвольным энергетическим разбиением и непосредственно связать этот процесс с

использованием многогрупповых программ расчета реакторов. Основу такой системы обработки информации составляет библиотека рекомендованных ядерных данных .

Существующие в настоящее время библиотечные форматы рекомендованных ядерных данных [2,4,3] позволяют хранить в удобном для практического использования виде большой объем разнообразной информации. В частности, они дают возможность включать в библиотеку данные по взаимодействию нейтронов и фотонов с ядрами различных веществ и данные по генерации фотонов. Такая информация позволяет решать на ЭВМ широкий круг задач, связанных с переносом нейтронов и фотонов.

Одни и те же ядерно-физические данные можно задать различным образом. Так, например, в резонансной области сечения могут быть представлены либо в виде детального энергетического хода, либо в виде задания резонансных параметров, либо, наконец, в форме подгруппового представления с разным числом подгрупп. Дифференциальные сечения упруго рассеянных нейтронов также могут быть заданы различными способами : в виде угловой зависимости или в виде разложения по полиномам Лежандра. Здесь также возможно подгрупповое представление данных.

Использование того или иного типа представления данных на практике определяется различными причинами : характером задачи, соображениями удобства, имеющимися в распоряжении программами и т.д. Поэтому желательно предусмотреть в библиотеке возможность хранения информации в различных представлениях. Для этой цели удобно ввести специальную характеристику – номер типа представления.

В настоящей работе обсуждаются форматы хранения рекомендованных ядерных данных для реакторных расчетов. Они представляют собой обобщения и дальнейшее расширение английских форматов, описанных в [2] и используемых в ряде зарубежных лабораторий. Важная особенность предлагаемых здесь форматов заключается во введении специальной классификации информации по типу представления. Это делает более гибкой систему хранения ядерных данных и позволяет полнее использовать возможности современных ЭВМ.

Излагаемый здесь формат хранения рекомендованных ядерных данных является дальнейшим развитием формата, предложенного в работе [6].

I. КЛАССИФИКАЦИЯ ЯДЕРНЫХ ДАННЫХ

Классификация библиотечных ядерных данных производится по трем признакам: по составу вещества, по типу происходящей в веществе реакции и по способу представленных данных.

Прежде всего, входящие в библиотеку данные подразделяются по веществам, к которым они относятся. Каждый набор данных для веществ определенного состава характеризуется идентифицирующим ядерным номером (ИЯН) и составляет более или менее самостоятельный массив информации. Данные, имеющие определенный ИЯН, классифицируются далее по возможным типам реакций, происходящих в этом веществе, с присвоением соответствующих номеров типа реакции (НТР). Наконец, ядерно-физические данные какого-либо фиксированного НТР классифицируются по способам их представления в библиотеке, отличаясь номерами типа представления (НТП).

I.I Идентифицирующий ядерный номер (ИЯН)

Каждый ИЯН может охватывать данные какого-либо определенного изотопа, элемента, химического соединения, смеси и т.д. Классификация по ИЯН позволяет также включать в библиотеку различные наборы данных для одного и того же вещества. Это могут быть, например, данные разных компиляций или данные, полученные из основных библиотечных данных с помощью различных обрабатывающих программ. Для включения таких данных в библиотеку им присваиваются новые значения ИЯН. Таким образом, ИЯН характеризует различные системы библиотечных данных как для различных веществ, так и для одного и того же вещества.

Нами принята следующая структура ИЯН. ИЯН представляет собой девятизначное целое число: $ИЯИ \equiv m_1 m_2 m_3 m_4 m_5 m_6 m_7 m_8 m_9$, последние три разряда $m_7 m_8 m_9$. которого используются для записи атомного номера изотопа A , а разряды m_5 и m_6 – для записи зарядового числа Z . Если набор данных относится к естественной смеси изотопов, то в разрядах $m_7 m_8 m_9$ проставляются нули. Если набор данных относится к химическому соединению, то нули проставляются в разрядах m_5 и m_6 , а разряды $m_7 m_8$ и m_9 используются для записи порядкового номера химического соединения.

Первые четыре разряда используются для обозначения порядкового номера набора данных в библиотеке оцененных данных.

Первую тысячу номеров решено сейчас оставить в резерве. Вторая тысяча номеров (с 1000 до 1999) отводится для записи наборов данных только об отдельных реакциях, или данных, относящихся к ограниченным энергетическим областям. Эта информация аналогична информации, хранимой в американской библиотеке ENDF/A и используется для создания полных наборов данных, необходимых для реакторно-физических расчетов. Для нумерации наборов данных такого типа отводится вторая тысяча номеров.

Номера наборов данных, относящихся к различным изотопам, элементам или химическим соединениям не могут совпадать между собой. Таким образом не может быть двух наборов данных с совпадающими первыми четырьмя знаками ИЯН (даже если последующие знаки различаются). Таким образом, пять последних разрядов ИЯН используются лишь для удобства идентификации наборов данных, тогда как первый разряд ИЯН определяет тип данных ($m_1 = 1$ неполный набор; $m_1 = 2$ – полный набор данных; смысл остальных возможных значений m_1 в настоящее время не фиксирован).

I.2. Номер типа реакции (НТР)

Данные, имеющие один и тот же ИЯН, подразделяются по типу происходящих в веществе реакций. Номер типа реакции (НТР) изображается пятизначным десятичным числом и разбивается на две части: двухзначный номер общей классификации (НОК) и следующий за ним трехзначный номер частной классификации (НЧК).

Конструирование НТР из НОК и НЧК придает системе классификации ядерных данных по реакциям большую гибкость. С помощью НТР можно, например, объединить в один набор, характеризуемый некоторым НЯН как нейтронные данные, так и данные по образованию фотонов и взаимодействию их с веществом. На практике однако при хранении этих трех типов данных часто бывает удобнее использовать три различных значения НЯН, тем более что диапазоны энергий для них, как правило, не совпадают.

Таким образом, появляется возможность различной компоновки данных в библиотеке с помощью НЯН и НТР. Такая возможность будет в дальнейшем расширена за счет введения номера типа представления (НТП).

I.3. Номер общей классификации (НОК)

Классификация по НОК делит данные с любым НЯН на группы в зависимости от их вида. Для нейтронных данных приняты следующие значения НОК:

01 – нейтронные сечения.
02 – угловые распределения вторичных частиц.
03 – энергетические распределения вторичных частиц.
04 – энерго-угловые распределения при рассеянии тепловых нейтронов.
05 – специальные величины для нейтронов ($\bar{\nu}$, α, η, β_i и т.д.).

Остальные значения НОК в настоящее время не идентифицированы. В частности, не идентифицированы НОК, определяющие константы взаимодействия фотонов с веществом в связи с отсутствием в нашем распоряжении такого рода рекомендованных данных.

I.4. Номер частной классификации (НЧК)

Номера частной классификации детализируют процессы ядерных взаимодействий. Каждый НЧК отождествляет один из таких возможных процессов, протекающих при столкновении нейтрона или фотона с веществом. Ниже дается спецификация НЧК для нейтронов, основанная на английской классификации.

001 – полное взаимодействие
002 – упругое рассеяние
003 – неупругое взаимодействие
004 – неупругое рассеяние (n, n')
005 –014 – неупругое рассеяние с возбуждением i -го уровня ядра-мишени ($i = 1, 2 \ldots, 10$)

015 – неупругое рассеяние с возбуждением прочих ("неразрешенных") уровней ядра-мишени

016 – ($n, 2n$)

017 – ($n, 3n$)

018 – деление $[(n,f)+(n,n'f)+(n,2nf)+\dots]$

019 – (n,f)

020 – $(n,n'f)$

021 – $(n,2nf)$

022 – $(n,n'd)$

023 – $(n,n'3d)$

024 – $(n,2nd)$

025 – $(n,3nd)$

026 – ($n, 2n$) изомерное состояние

027 – 100 – резервируются для других возможных процессов, приводящих к возникновению вторичных частиц того же типа, что и первичные

101 – полное поглощение (все процессы, не приводящие к вылету частиц типа первичных)

102 – (n,γ)

103 – (n,p)

104 – (n,d)

105 – (n,t)

106 – (n,He^3)

107 – (n,α)

108 – $(n,2\alpha)$

109–150 – резервируются для других возможных процессов, не приводящих к возникновению вторичных частиц того же типа, что и первичные

151 – 200 – в английской библиотеке используются для классификации информации по разрешенным и статистическим резонансам. Детализация НЧК здесь непосредственно связана с формой представления данных. Нами эти НЧК пока не используются.

201 – 999 – резервируются для разного рода других данных, которые могут потребоваться или будут появляться в дальнейшем.

Как видно, сольшое число НЧК пока оставлено свободным для удовлетворения дальнейших потребностей библиотеки рекомендованных ядерных данных.

В английской классификации НЧК = 201–208 используются для идентификации таких характеристик как транспортное сечение, сечение увода, $\sqrt{\sigma_f}$ и некоторых других производных величин. Номера с 301 по 450 отводятся для параметров типа ($\bar{\sigma}_k \bar{E}_k$), характеризующих скорость энерговыделения, где $\bar{E}_k$ – средняя энергия, выделяющаяся в процессе k. Эти величины также являются производными от величин с НЧК от 001 до 150; соответствующий процесс идентифицируется путем вычитания из этого НЧК числа 300. Таким образом, например, НЧК = 301 означает параметр скорости полного энерговыделения, а НЧК = 302 – аналогичный параметр в случае упругого рассеяния.

Производные величины обычно не содержатся в библиотеке рекомендованных ядерных данных, но могут быть легко получены с помощью особых программ. Естественно поэтому не фиксировать для них НЧК (по крайней мере, в настоящее время). Такого рода величины, по-видимому, удобнее включить в библиотеку групповых констант, которая будет создаваться на основе настоящей библиотеки детальных данных с помощью специальных обрабатывающих программ.

Спецификация реакций такова, что НЧК позволяет однозначно установить вид продуктов реакции. Так, например, для ядра C^{12} реакция $C^{12}(n,n')3\alpha$ имеет НЧК = 023, в то время как реакция $C^{12}(n,n')C^{12*}(\gamma)C^{12}$ - НЧК = 5, если рассматривается первое возбужденное состояние 4,43 Мэв. Аналогично для U^{238} НЧК = 016 означает, что конечными продуктами реакции будут $Np^{237}+2n$. Таким образом, при любом ядерном превращении имеется возможность по НЧК определить как вид остаточного ядра, так и вид вылетающих частиц.

Примеры НТР

01001 - полное сечение взаимодействия нейтронов;
01002 - сечение упругого рассеяния нейтронов;
02018 - угловые распределения мгновенных нейтронов деления;
03016 - распределение по энергиям нейтронов, возникающих в результате реакции ($n,2n$);
05018 - среднее число нейтронов на деление, $\bar{\nu}$.

I.5. Номер типа представления (НТП)

Поскольку данные могут быть представлены в библиотеке различными способами, они классифицируются по номеру типа представления (НТП). Введение НТП позволяет реализовать различные способы задания данных в пределах одного и того же НТР, существенно расширяя тем самым возможности системы хранения рекомендованных ядерных данных.

Можно указать на следующие способы представления данных в библиотеке:

- представление данных в виде детальной энергетической или угловой зависимости;
- параметрическое представление, например, с помощью задания коэффициентов разложения по полиномам Лежандра в случае угловых распределений;
- подгрупповое представление данных [5] с различным числом подгрупп нейтронов.

При подгрупповом представлении нейтроны с данной энергией разбиваются на некоторое количество (N) подгрупп. Каждая такая подгруппа (n), характеризуемая своим значением сечения σ_n, имеет долю a_n, так что

$$\sum_{n=1}^{N} a_n = 1.$$

Подгрупповое представление является удобным способом задания данных в области неразрешенных резонансов. В этом случае a_n может рассматриваться как вероятность того, что полное сечение при рассматриваемой энергии E будет равно σ_n. Подгрупповое представление может применяться также и в случае разрешенных резонансов, если нет необходимости иметь детальный ход ядерных данных в этом энергетическом интервале.

Настоящий формат предполагает, что между полным и парциальными подгрупповыми сечениями существует полная корреляция, т.е. нейтроны данной подгруппы n имеют не только одинаковое полное сечение σ_n, но и одинаковые парциальные сечения σ_{rn}. Если использование этого приближения не оправдано, метод подгрупп становится непрактичным.

Для угловых и энергетических распределений вторичных частиц могут быть использованы различные законы представления данных, отражающие те или иные механизмы протекания данного ядерного процесса. Классификацией НТП предполагается конструирование угловых и энергетических распределений в виде суперпозиции таких законов с заданными вероятностями для каждого из них.

Кроме этого, с введением НТП появляется возможность более гибкой компоновки данных, хранящихся в библиотеке. В частности, становится возможным изменять по желанию количество и порядок подчиненности переменных (параметров), от которых зависят представляемые библиотечные данные.

НТП конструируется таким образом, чтобы можно было осуществить на практике наряду с различными способами задания данных (в дискретных точках, параметрически и т.д.) такие различные порядки старшинства переменных, от которых зависят представляемые данные. Структура НТП, вообще говоря, зависит от НТР и определяется НОК. Принимается, что для любого НОК в качестве НТП достаточно взять трехзначное десятичное число

$$НТП = n_1 n_2 n_3 ,$$

разряды которого в зависимости от НОК могут иметь различный смысл. В ряде случаев приводится дополнительная информация, уточняющая смысл НТП. Идентификация разрядов НТП и дополнительной информации будет рассмотрена при обсуждении форматов представления данных для соответствующих НОК.

I.6. Представление сечений с помощью резонансных параметров.

В настоящее время определяется лишь формат записи данных для брейт-вигнеровских параметров резонансов. Форматы записи параметров, используемых в других формулах, будут разрабатываться по мере того, как будут составляться и использоваться для расчета сечений программы вычислений по другим формулам.

При разработке нашего формата мы опирались на формат, принятый в английской библиотеке резонансных параметров *RPL* [7], видоизменив его в соответствии с общими требованиями формата библиотеки СОКРАТОР. Внесенные изменения, однако, таковы, что числовые данные о резонансных параметрах могут быть полностью переведены из одного формата в другой с помощью

простой программы. Хранение вспомогательной информации (ссылка на отчет по оценке, дата и место оценки и др. алфавитная информация) в формате основной библиотеки СОКРАТОР, в отличие от RPL, не предусматривается; эта информация может быть помещена в параллельную основной библиотеке библиотеку текстовых комментариев.

I.6.I. Формула Брейта-Вигнера

Сечение рассеяния:

$$\sigma_{nn}(E)=\pi\lambda^2\sum_{J,\pi}g_J\Big[\sum_{\ell=|I-s|}^{I+s}\Big\{\sin^2\varphi_{cJ}+\sum_{r=1}^{N}B_r(E)\Big[\Gamma_{rn}\Gamma_{rnc}\cos 2\varphi_{cJ}-2\Gamma_{rx}\Gamma_{rnc}\sin^2\varphi_{cJ}(I)$$
$$+2(E-E_r')\Gamma_{rnc}\cdot\sin 2\varphi_{cJ}\Big]\Big\}+\sum_{r=1}^{N}B_r(E)\Big[\Gamma_r\cdot\alpha_r-2(E-E_r')B_r\Big]\Gamma_{rn}+\sigma_{nn}^{плав}(E)$$

Сечение реакции (n,R):

$$\sigma_{nR}(E)=\pi\lambda^2\sum_{J,\pi}g_J\sum_{r=1}^{N}\Gamma_{rn}\Gamma_{rR}B_r(E)+\sigma_{nR}^{плав}(E) \qquad (2)$$

Полное сечение:

$$\sigma_{nT}(E)=\sigma_{nn}(E)+\sum_{R}\sigma_{nR}(E) \qquad (3)$$

Здесь использованы следующие обозначения:

$$B_r(E)=\frac{1}{(E-E_r')^2+\Gamma_r^2/4} \qquad (4)$$

$$\alpha_r=\frac{1}{2}\cdot\sum_{s\neq r}\frac{\Gamma_{sn}(\Gamma_s+\Gamma_r)}{D_{sr}} \qquad (5)$$

$$\beta_r=\sum_{s\neq r}\frac{\Gamma_{sn}(E_s'-E_r')}{D_{sr}} \qquad (6)$$

$$D_{sr}=(E_s'-E_r')^2+\frac{1}{4}(\Gamma_s+\Gamma_r)^2 \qquad (7)$$

$\Gamma_{rn}\equiv\Gamma_{rn}(E)=\sum_{\ell=|I-s|}^{I+s}\Gamma_{rnc}(E)$ – полная нейтронная ширина (8)

$\Gamma_{rx}\equiv\Gamma_{rx}(E)=\sum\Gamma_{rR}(E)$ – ширина неупругих взаимодействий (9)

$\Gamma_r\equiv\Gamma_r(E)=\Gamma_{rn}(E)+\Gamma_{rx}(E)$ – полная ширина (10)

Эффективная резонансная энергия E_r' :

$$E_r' = E_r + \frac{1}{2}\sum_{\ell=\ell_1}^{L_2}\left[\delta_\ell(|E_r|) - \delta_\ell(E)\right]\Gamma_{rn\ell}(|E_r|)/P_\ell(|E_r|) + \\ + \frac{1}{2}\sum_{a}\left[\delta_a(|E_r|) - \delta_a(E)\right]\cdot\Gamma_{ra}(|E_r|)/P_a(|E_r|) \qquad (II)$$

Для $\ell=0$ δ_ℓ не зависят от E . Обычно δ_a берутся постоянными и для других реакций.
Если, как здесь сделано, задавать δ при $E = E_r$, то $E_r'(E_r) = E_r$ всегда, а как правило, $E_r' = E_r$ и при других E.

Первая сумма (по J и π) берется по всем системам уровней, которые могут давать вклад в сечение.

Сумма по ℓ берется по всем орбитальным моментам нейтронов, которые могут образовывать состояния с данными J и π ;

$$L_1 = \min\left\{|J - |I - \tfrac{1}{2}||;\ |J - I - \tfrac{1}{2}|\right\}, \qquad (I2)$$

если

$$(-1)^{L_1} = \pi\cdot\pi_I, \qquad (I3)$$

где π_I - четность основного состояния ядра мишени.
Если условие по четности (I3) для L_1 , определенного согласно (I2), не выполняется, то L_1 не единицу больше, чем следует из (I2).

$$L_2 = J + I + \frac{1}{2}, \qquad (I4)$$

если

$$(-1)^{L_2} = \pi\cdot\pi_I \qquad (I5)$$

или на единицу меньше, если условие (I5) не выполняется.

Из-за условия сохранения четности

$$(-1)^{\ell} = \pi\cdot\pi_I \qquad (I6)$$

значение ℓ в сумме при переходе от одного члена к другому меняется на 2.

Поскольку обычно

$$\Gamma_{rn\ell_1} \gg \Gamma_{rn}(L_1+2) \gg \ldots \gg \Gamma_{rn\ell_2},$$

(исключением являются высокие энергии, когда $ka \geq 1$), то, как правило, можно положить $L_2 = L_1$.

Предпоследний член в (I) учитывает некорезонансную интерференцию в рамках приближения Брейта-Вигнера. Этот учет точен, если выполняется хотя бы одно из следующих условий:

а) резонансы хорошо разделены и интерференция несущественна;

б) существенен только один нейтронный канал (взаимодействуют только S-нейтроны или также и нейтроны с высокими моментами, но спин ядра-мишени $I = 0$).

Фазовый сдвиг φ_{cy} определяется через радиус канала $a_{cy}(E)$: $\varphi_{cy} = k a_{cy}$. Здесь

$$k = 2{,}19685 \cdot 10^{-3} \sqrt{E}\ \frac{M}{M+1.08665}\quad (\text{барн})^{-1/2}$$

M – масса ядра (принимая массу $C^{12} = 12$),

$$a_{cy} = a + \Delta a_{cy}(E)$$

есть эффективный радиус ядра для данного канала. Если зависимость a_{cy} от энергии существенна, то в библиотеке приводится эта зависимость для a_{cy} (а не для Δa_{cy}).

Последние члены в (1) и (2) описывают вклады далеких резонансов, а также пропущенных уровней. Эти сечения либо задаются в точках, либо рассчитываются по средним резонансным параметрам. В формуле (1) этот член может быть корректно учтен через эффективный радиус a . Для этого необходимо, однако, чтобы резонансные параметры определялись с учетом межрезонансной интерференции. Если это не так, то $\sigma_{nn}^{\text{плав}}(E)$, по сути дела, описывает результат интерференции многих уровней.

6.2. Приближения к формуле Брейта-Вигнера

а) Пренебрежение членом, описывающим межрезонансную интерференцию. Это, вообще говоря, ведет к появлению отрицательных сечений между резонансами, если не добавлено плавное сечение. Резонансные параметры определяются, как правило, именно в этом приближении. Поскольку, однако, при этом рассматриваются лишь области резонансных пиков, найденные в этом приближении параметры достаточно точны. Радиус ядра при этом получается, однако, неточно и нуждается в поправке для того, чтобы можно было использовать эти параметры в строгой формуле.

б) Приближенный учет межрезонансной интерференции, обеспечивающий положительность решения. Этот метод реализован в программе УРАН [8] . Он заключается в том, что φ_{cy} в каждой точке E в окрестности данного резонанса r заменяется на φ_{cy}^{*} , определенное так, чтобы

$$4\sin^2\varphi_{cy}^{*}(E) = 4\sin^2\varphi_{cy} + \sum_{\substack{s=r-5\\ s\neq r}}^{r+5} B_s(E)\Big[\Gamma_{sn}\Gamma_{sne}\cos 2\varphi_{cy} - 2\Gamma_{sx}\Gamma_{sne}\sin^2\varphi_{cy} + 2(E-E_s')\Gamma_{sne}\sin 2\varphi_{cy}\Big]$$

Расчет производится по формуле (1) с опущенным межрезонансным членом, но с использованием $\varphi_{cy}^{*}(E)$ вместо φ_{cy} , что и обеспечивает положительность сечения.

в) Пренебрежение факторами сдвига. Поскольку $\delta_\ell(E)$ -константа, это важно лишь для $\ell > 0$ и лишь вдали от резонанса. Поэтому параметры, определенные в этом приближении, могут использоваться в точной формуле непосредственно.

г) Приближения для области низких энергий:

$$\sin^2\eta_\ell \approx k^2a^2, \quad \eta_\ell = 0 \quad \text{для } \ell > 0.$$

Если это приближение использовалось при определении параметров в той области, где оно пригодно, параметры годятся и для использования их в общей формуле.

д) Пренебрежение фактором $\frac{M}{M+1.0865}$ в выражении для k. Если параметры определены в этом приближении, то и в исходных данных значение M должно быть положено достаточно большим, с тем чтобы этот множитель был близок к единице. Тогда такие параметры можно будет использовать и в общей формуле.

Проницаемости и фазовые сдвиги должны определяться одним из трёх путей.

I) для нейтронных каналов P_ℓ и S_ℓ рассчитываются для прямоугольной ямы. В частности,

$$P_0 = 1;$$

$$P_1 = \frac{(kR)^2}{1+(kR)^2};$$

$$P_2 = \frac{(kR)^4}{9+3(kR)^2+(kR)^4};$$

$$P_3 = \frac{(kR)^6}{225+45(kR)^2+6(kR)^4+(kR)^6}$$

Для других реакций берется $P_\ell(E) = 1$, $\delta_\ell(E) = 0$

2) P_ℓ, δ_ℓ, P_ℓ и δ_ℓ могут быть заданы с табличной форме в функции энергии нейтронов, будучи определены эмпирически или рассчитаны по той или иной теоретической модели (например, для случая реакций с испусканием заряженных частиц).

3) фазовые сдвиги и проницаемости рассчитываются по некоторому алгоритму, номер которого указан в библиотечных данных.

II. ПРЕДСТАВЛЕНИЕ ДАННЫХ НА КАРТАХ

Содержащаяся в библиотеке информация по ядерным данным предполагается набитой на символических картах. Каждая такая карта содержит определенное количество основной и служебной информации. Основная информация включает в себя собственно ядерные данные в виде таблиц числовых значений и вспомогательные данные, играющие роль заголовков к таблицам ядерных дан-

ных в кодированном числовом виде. Служебная информация состоит из разного рода меток, позволяющих отличать карты друг от друга. Наличие меток облегчает также программную обработку библиотечных данных.

В качестве символической карты берется стандартная 80-колонковая перфокарта. Однако в зависимости от особенностей внешних устройств ЭВМ разметка ее производится различным образом. Сделаем некоторые общие замечания, касающиеся разметки карт и кодирования располагаемой на них информации.

В том случае, когда для кодирования информации используется 960 позиций (12 строк х 80 колонок), разметка перфокарты может иметь, например, такой вид: 6 полей (по 11 колонок в каждом), разделенных между собой пустой колонкой, отводятся для основной информации (поля данных), а колонки с 73 по 80 – для служебной информации (поле меток). Такой вид разметки принят в английской библиотеке рекомендованных ядерных данных.

При использовании вводных устройств машин типа М-20 удобнее принять другой вид разметки перфокарты. В этом случае под основную информацию отводится 6 верхних строк, а в следующих строках размещается служебная информация.

Оба эти типа разметки оказываются эквивалентными в смысле расположения набитой на символической карте информации при выводе ее на печать с помощью соответствующих внешних устройств. Роль основной структурной единицы играет либо поле, либо строка соответственно в первом и втором случаях. В каждом поле (строке) фиксируется одно машинное слово (одно число). Алфавитная кодировка в основной библиотеке не используется[x]. Вид представления чисел определяется их смысловой нагрузкой. Все ядерные данные представляются в двоично-десятичном коде с плавающей запятой.

Во втором случае возможна также несколько иная форма разметки перфокарты. Учитывая тот факт, что число значащих цифр в числовых данных, как правило, невелико, служебную информацию можно хранить параллельно с основной, отведя под нее, например, три последних десятичных разряда (третий адрес) каждой из шести строк с основными данными. При такой разметке на одной стандартной перфокарте помещается две символических карты.

Для любого вещества данные, характеризуемые некоторым ИЯН, составляют замкнутый массив информации в том смысле, что эта информация может быть использована в дальнейшем самостоятельно без привлечения каких-либо других массивов с аналогичными данными для этого вещества. Комплект с таким замкнутым набором данных будем в дальнейшем называть файлом (от английского $f i \ell e$ – картотека). Каждому файлу приписывается определенный библиотечный номер (БНФ), который и проставляется в первых четырех разрядах ИЯН.

Файл разбивается на секции по числу типов реакций, имеющих место для вещества с данным ИЯН. Каждая секция включает в себя карты с ядерными данными определенного НТР. Одному и тому же типу реакции в разных файлах будут соответствовать, вообще говоря, различные секции. Соответствие меж-

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x) Предполагается, что параллельно с основной библиотекой, содержащей числовые данные, будет существовать библиотека текстовых комментариев к каждому файлу . Формат этой библиотеки в настоящее время не разработан.

ду номером секции и НТР устанавливается на специальных заголовочных картах, занимающих нулевую секцию файла. Внутри каждой секции карты имеют последовательную нумерацию. Нумерация секций в пределах каждого файла автономна.

Порядок следования секций для нейтронных данных определяется, в первую очередь, НЧК, а при одинаковых НЧК величиной НОК.

Примеры нумерации секций

Номер секции	НТР	Наименование данных
00		Заголовочная информация
01	01001	Полное сечение взаимодействия нейтронов.
02	01002	Сечение упругого рассеяния нейтронов
03	02002	Угловое распределение упруго рассеянных нейтронов
04	01003	Сечение неупругих взаимодействий.
05	01004	Сечение неупругого рассеяния
06	01005	Сечение неупругого рассеяния с возбуждением 1-го уровня ядра
07	02005	Угловое распределение нейтронов, неупруго рассеявшихся с возбуждением 1-го уровня ядра.
08	03005	Энергетическое распределение нейтронов, неупруго рассеявшихся с возбуждением 1-го уровня ядра.

Как содержание, так и само расположение основной информации на картах зависит от НТР (главным образом от НОК), а также от НТП, и будут рассмотрены в дальнейшем подробно. Что касается служебной информации, то она включает в себя ИЯН (БНФ), номер секции, порядковый номер карты в секции и также циклическую сумму информации, пробитой в первых восьми строках перфокарты.

В соответствии с наиболее распространенным сейчас в СССР типом карточных перфораторов и вводных устройств нами принята построчная разметка перфокарт.

В первых шести строках перфокарты записывается основная информация, всегда записываемая в двоично-десятичном коде с плавающей запятой (в том числе и целые числа). Порядок представления основной информации на перфокартах описан ниже (раздел Е).

В седьмой строке набивается девятизначное целое число, два младших разряда которого представляют собой номер секций, в которой расположены данные рассматриваемого типа[x)], четыре старших разряда используются для записи четырех старших разрядов ИЯН (библиотечный номер файла - БНФ) в рассмотренном выше формате. 5-й, 6-й и 7-й разряды не используются.

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x)Связь между номером секции и НТР определяется в первой заголовочной секции файла.

В восьмой строке пробивается номер перфокарты в секции в виде числа с плавающей запятой. Нумерация карт каждой секции начинается заново с перфокарты № I (содержащей всегда заголовочную информацию для данной секции).

Девятая строка содержит циклическую сумму чисел, записанных в первых восьми строках, однако признак контрольной суммы в этой строке не пробивается. Последнее позволяет непрерывно вводить в ЭВМ массив, состоящий из многих карт. После ввода данных с помощью контрольной суммы может быть проверена правильность ввода информации на каждой перфокарте и выявлены дефектные перфокарты.

III. ФОРМАТЫ ПРЕДСТАВЛЕНИЯ ЯДЕРНЫХ ДАННЫХ В БИБЛИОТЕКЕ

Так как характер ядерных данных определяется видом реакции, форматы представления этих данных в библиотеке зависят от НТР, в первую очередь, от НОК. Форматы, естественно, будут зависеть также от КТЦ. Прежде чем рассматривать конкретные форматы для разных НОК, сделаем некоторые замечания общего характера.

Область энергий, рассматриваемых для данного НТР, в случае необходимости разбивается на некоторое число интервалов. При разбиении нужно учитывать ряд соображений,включая следующие:

I. На отдельных участках данные пренебрежимо малы или равны нулю (например, сечения до порога реакции).

2. В некоторых интервалах соответствующие данные не зависят от энергии или представляются одинаковым образом.

3. В разных энергетических интервалах данные имеют различные представления или различные температурные зависимости.

Разбиение энергетической области на интервалы позволяет в некоторых случаях избежать дублирования результатов. При этом по возможности необходимо стремиться к минимальному числу интервалов. Для различных НТР в пределах одного НЯИ число интервалов может быть разным. Например, полное сечение и сечение порогового процесса будут иметь разное количество интервалов. Желательно иметь, там где это возможно, совпадающие энергетические интервалы для полного сечения и составляющих его парциальных сечений. Это может облегчить обнаружение грубых ошибок с помощью специальных программ.

Обычно ядерные данные задаются в дискретных энергетических точках. Если,однако,в некотором интервале энергий данные постоянны, они могут быть заданы для всего этого интервала в целом. Такая возможность осуществляется с помощью специальных форматов, предусмотренных классификацией НТП.

В тех случаях, когда ядерные данные задаются для дискретных значений переменных, от которых эти данные зависят, выбор соответствующих значений

независимых переменных должен удовлетворять определенным требованиям. Именно значения переменных должны выбираться с таким условием, чтобы значения самой функции при любых промежуточных значениях аргументов можно было с достаточной для практики точностью получить с помощью интерполирования между соседними, имеющимися в библиотеке, значениями. В некоторых случаях целесообразно интерполировать в логарифмическом масштабе (сечения, специальные величины для нейтронов). Способ интерполяции и порядок интерполяционного многочлена для тех или иных записываемых в библиотеку массивов данных определяются оценщиками с учетом возможностей имеющихся обрабатывающих программ и указывается в качестве дополнительной информации в заголовках НТП.

Закон интерполяции задается в библиотеке девятизначным числом ИНТ

$$\text{ИНТ} \equiv i_1'' i_2'' i_3'' i_1' i_2' i_3' i_1 i_2 i_3$$

С помощью числа ИНТ может быть определен закон интерполяции для функции одной, двух и трех переменных.

Три младших разряда $i_1 i_2 i_3$ определяют закон интерполяции по младшей переменной; три следующих разряда – $i_1' i_2' i_3'$ – для следующей по старшинству; три старших разряда – $i_1'' i_2'' i_3''$ – для старшей переменной. Порядок старшинства переменных определяется НТП (см. ниже).

В каждой тройке чисел $i_1 i_2 i_3$ разряд i_1 определяет способ интерполяции. $i_1 = 1$ означает линейную интерполяцию. Смысл других значений i_1 в настоящее время не фиксирован. Два следующих разряда определяют масштаб, в котором должна проводиться интерполяция: i_2 – по оси ординат (масштаб интерполируемой функции), i_3 – по оси абсцисс (масштаб аргумента).

Масштаб определяется следующей таблицей:

Значение i_2 или i_3	Масштаб по соответствующей оси
0	линейный
1	логарифмический
2	корневой
3	косинусоидальный

Смысл остальных значений i_2 и i_3 в настоящее время не фиксирован.

Примеры: 1. Функция одной переменной $\sigma(E)$.

ИНТ = ++ 09 111 000 000

означает линейную интерполяцию ($i_1'' = 1$) в двойном логарифмическом масштабе ($i_2'' = i_3'' = 1$). Энергия E здесь является единственной и поэтому старшей переменной.

2. Функция двух переменных – спектр вторичных нейтронов в зависимости от энергий падающих нейтронов: $f(E_0, E)$.

ИНТ = ++ 09 100 000 000

означает линейную интерполяцию величины f по каждой из переменных в линейном масштабе.

3. Функция трёх переменных – суперпозиция угловых распределений: $f(E,\mu) = \sum_{k=1}^{n} a_k(E) f_k(E,\theta)$ ($a_k(E)$ могут иметь, например, смысл зависящих от энергии долей подгрупп, а f_k – подгрупповых угловых распределений).

ИНТ = ++ 09 101 001 003

означает при старшинстве переменных a, E, θ, что $a_k(E)$ должно интерполироваться линейно на графиках зависимости a_k от $\ell_n E$ ($i_1''=1, i_2''=0, i_3''=1$), f_k должны интерполироваться по энергии аналогичным образом ($i_1'=1, i_2'=0, i_3'=1$) и линейно по косинусу угла θ ($i_1=1, i_2=0, i_3=3$).

Когда важна температурная зависимость ядерных данных, указывается значение температуры, которой они соответствуют. Если зависимость данных от температуры T может быть учтена в процессе расчетов аналитически, задания одного значения T оказывается достаточным. В противном случае результаты приводятся при нескольких различных температурах таким образом, чтобы методом интерполирования можно было получить данные для любой нужной температуры.

Например

ИНТ = ++ 09 102 000 000

означает, что интерполяция должна вестись линейно на графике зависимости сечения от $\sqrt{T}$ ($i_1''=1, i_2''=0, i_3''=2$).

Спецификация НТР такова, что она позволяет однозначно идентифицировать как вид остаточного ядра, так и вид продуктов любой рассматриваемой ядерной реакции. В частности, вполне однозначно определяется число вторичных частиц, образующихся в результате реакции. Поскольку, однако, некоторые данные, например экспериментальные данные по угловым и энергетическим распределениям, могут быть известны не для каждой вторичной частицы продуктов ядерной реакции в отдельности, а возможно, в некоторых случаях лишь для определенных групп частиц продуктов, в соответствующих форматах предусматривается специальное условное число, отождествляющее группы частиц, для которых такие данные задаются.

Библиотечные форматы предусматривают хранение информации в виде отдельных массивов, каждый из которых, в свою очередь, также может включать в себя массивы меньшего объема. Распределение данных по массивам производится на основе наличия у них тех или иных общих признаков, например, это могут быть данные одного и того же НТР или НТП, данные, относящиеся к одному и тому же энергетическому интервалу, температуре и т.д.

Все массивы снабжены специальными заголовками. Любой заголовок содержит характеристику массива и сведения о количестве и, возможно, расположении непосредственно подчиненных ему более мелких массивов. Это позволя-

ет иметь общее представление о внутреннем содержании .массива по одному лишь заголовку, без распаковки самого массива.

Каждый заголовок начинается с новой карты. Формат для любого НОК включает в себя следующие заголовки:

- заголовок типа реакции,
- заголовок энергетических интервалов,
- заголовки температуры (НОК = 01, НОК = 04, НОК = 05) или группы вторичных частиц (НОК = 02, НОК = 03),
- заголовки типов представлений.

Порядок следования остальных, внутренних по отношению к данному типу представления, заголовков определяется НТП. К ним относятся, например, заголовки энергии, подгруппы нейтронов и т.п.

Поле или строка в дальнейшем называются позицией. При описании конкретных форматов карты нумеруются римскими цифрами, а позиции карты, занятые под основную информацию - арабскими. В позициях, не занятых информацией, пробиваются нули.

II.1. Заголовок файла

Заголовок файла занимает нулевую секцию и устанавливает соответствие между номером секции, номером типа реакции и количеством занимаемых секций карт. Формат заголовка имеет вид:

Тип карты

I. 1. НЯИ.
2. Полное число карт в этом файле, включая карты заголовка.
3. Число карт в нулевой секции.
4. Атомный номер Z элемента (нуль для химических соединений и смесей).
5. Атомный или молекулярный вес A.
6. Число различных НТР, имеющих место для данного вещества.

I. 1. Номер секции.
2. Соответствующий НТР.
3. Число карт в этой секции.

В случае необходимости информация переходит на последующие позиции этой и следующих за ней карт в формате позиций I-3 карты типа II.

II.2. Нейтронные сечения (НОК = 01)

В библиотеке числовые значения сечений хранятся вместе с соответствующими значениями переменной, от которой они зависят. В качестве переменной могут выступать энергия, температура, номер подгруппы и др. Данные по сечениям приводятся в порядке естественного следования значений переменной. Для энергии и температуры это означает их монотонный рост. Нумерация подгрупп производится в порядке возрастания сечений. В принятых форматах энергии задаются в Мэв, температуры – в градусах К, а сечения в барнах.

Значения энергии и температуры выбираются с учетом возможности получения сечений методом интерполирования. Для сечений очень часто интерполирование производится в логарифмической шкале. В этом случае требуется, чтобы во всех точках, включая границы интервала, были заданы отличные от нуля значения сечений.

Классификацией НТП предусматривается также задание сечения сразу для всего энергетического интервала, если оно в этом интервале постоянно.

Полное сечение и составляющие его парциальные сечения желательно задавать в одних и тех же точках. Это может облегчить процесс обнаружения грубых ошибок в данных по сечениям с помощью специальных программ проверки.

II. 2.I. Классификация НТП для НОК = 01

Старший разряд НТП определяет способ задания данных по сечениям в соответствии со следующей таблицей

n_1	Способ задания сечений
I	В дискретных точках по E и T в подгрупповом представлении
2	В дискретных точках по E в подгрупповом представлении с параметрическим описанием температурной зависимости подгрупповых параметров.
3	Параметрически с помощью резонансных формул для разрешенных резонансов.
4	Параметрически с помощью статистических данных для неразрешенных резонансов.

Последующие значения n_1 (5–9) резервируются для новых способов задания, если таковые будут появляться.

Смысловая нагрузка младших разрядов НТП, вообще говоря, зависит от n_1. Для n_1 = I они имеют следующий смысл:

n_2 – означает число переменных или параметров, от которых могут зависеть сечения,

n_3 – определяет порядок старшинства этих параметров друг относительно друга.

В случае двух параметров (энергия E и номер подгруппы i) идентификация младших разрядов НТП определяется таблицей

$n_2\,n_3$	Старшая переменная	Младшая переменная
0I	-	-
II	E	-
I2	i	-
2I	E	i
22	i	E

Случай $n_2\,n_3$ = 0I соответствует заданию сечения сразу для всего энергетического интервала.

Для n_1 = 2 формат карт и классификация n_2 и n_3 в настоящее время не определены.

Для n_1 = 3 второй разряд НТП - n_2 определяет тип резонансной формулы. В соответствии с RPL [7] принимаем:

n_2 = I для формулы Брейта-Вигнера;
n_2 = 2 для формул, основанных на приведенной R -матрице (формула Райха-Мура);
n_2 = 3 для R -матричной формулы Бриссендена-Берстона
n_2 = 4 для S -матричной формулы Адлеров;

r_3 равное нулю означает, что резонансные параметры в секции для данного НЧК не приводятся; брать их надо из секции для полного сечения (НЧК=00I).

В секции для полного сечения значение n_3 = 0 для наименьшей из приводимых температур недопустимо. Остальные значения n_3 = I,2,...,9 означают номер приближения к общей формуле, которое рекомендуется использовать при расчетах по заданным параметрам.

n_3 = I всегда означает, что параметры рассчитаны на применение общей формулы. При $n_2 = 1$, $n_3 = 2$ означает, что рекомендуется применять приближение, реализованное в программе УРАН [8] . Смысл других значений n_3 в настоящее время не идентифицирован.

III. 2.2. Формат карт для НОК = 0I при задании сечений в дискретных точках по E и T (n_1 = I)

I. I. НТР.
2. Число энергетических интервалов (ΔE) для этого НТР.
3. Q - энергия реакции (Мэв).
4. } Резервируются для дополнительной информации этого НТР.
5. }
6. }

II. 1. $E_н$ – нижняя граница ΔE .
2. $E_в$ – верхняя граница ΔE .
3. Число карт для представления сечений в этом ΔE , включая настоящую карту.
4. Число температур T, рассматриваемых в этом ΔE .
5. Число ИНТ , определяющее закон интерполяции по температуре.
6. Резервируются для дополнительной информации в этом ΔE .

III. 1. Температура T, которой соответствуют сечения.
2. Число НТП для сечений при этой температуре.
3. Число карт для представления сечений при этой T, включая настоящую карту.
4.
5. } Резервируются для дополнительной информации при этой T.
6.

Формат последующих карт зависит от НТП.

1) сечение в данном ΔE не зависит от энергии (одна подгруппа).

IV. 1. НТП = 101.
2. Значение сечения σ .

2) сечение зависит от энергии (одна подгруппа)

IV. 1. НТП = 111.
2. Число значений энергии.
3. Число карт для этого НТП.
4. Число ИНТ , определяющее закон интерполяции сечения по энергии
5. E.
6. $\sigma(E)$.

В случае необходимости информация переходит на следующие карты в формате позиции 5–6 карты IV.

3) подгрупповое представление структуры сечения для всего ΔE

IV. 1. НТП = 112.
2. Число подгрупп.
3. a_1.
4. σ_1.
5. a_2.
6. σ_2.

В случае необходимости информация переходит на последующие карты в формате позиций 3–4 карты IV.

4) сечение зависит от энергии. Подгрупповое представление структуры сечения при фиксированных E .

IV. 1. НПП = 121 .
2. Число значений E.
3. Число карт для представления сечений этим НПП, включая настоящую карту.
4. Число подгрупп (если оно не зависит от E).
5. Число ИНТ, определяющее закон интерполяции по энергии.
6. Число, определяющее какая величина должна подвергаться усреднению:

а) если возможно непосредственное усреднение σ_i и σ_i для некоторых интервалов ΔE или Δu , лежащих внутри интервала $[E_н, E_к]$, то в этой позиции приводится либо максимальный интервал летаргии, для которого такое усреднение еще позволяет с достаточной точностью определить подгрупповые характеристики (предполагается, что этот интервал должен быть меньше 2) либо максимальный энергетический интервал, взятый со знаком минус (минус и является признаком того, что интервал задан в масштабе энергии);

б) если в этой позиции стоит 2 , то усреднение должны подвергаться функции пропускания

$$T_t(t) = \frac{1}{\Delta E}\int_{\Delta E} e^{-\sigma_t(E)\cdot t}\cdot f(E)\cdot dE \qquad \text{(если } \sigma \text{ – полное сечение)}$$

$$T_R(t) = \frac{1}{\Delta E}\int_{\Delta E} \sigma_R(E)\, e^{-\sigma_t(E)\cdot t}\cdot f(E)\cdot dE \qquad \text{(если } \sigma = \sigma_R \text{ – сечение реакции типа R).}$$

($f(E)$ – спектр, по которому производится усреднение).

Подгрупповые параметры для интервала ΔE определяются затем из условия аппроксимации $T_t(t)$ и $T_R(t)$ суммой минимального числа экспонент, обеспечивающего заданную точность аппроксимации:

$$T_t(t) \approx \sum_{k=1}^{p} a_k e^{-\beta_k t}$$

$$T_R(t) = \sum_{k=1}^{p} a_k \beta_{k-1} e^{-\beta_k t}$$

в) если в этой позиции стоит 3 , то рекомендуемый метод получения подгрупповых характеристик для интервалов состоит в вычислении моментов сечения $\langle\sigma_t\rangle, \langle\sigma_R\rangle, \langle 1/\sigma_t\rangle, \langle 1/\sigma_t^2\rangle, \langle\sigma_R/\sigma_t\rangle$ (если число подгрупп = 2) или также $\langle\sigma_t^2\rangle, \langle 1/\sigma_t^3\rangle$ и $\langle\sigma_R\sigma_t\rangle$ (если число подгрупп = 3), или, наконец, также $\langle\sigma_t^3\rangle, \langle 1/\sigma_t^4\rangle$ и $\langle\sigma_R\sigma_t^2\rangle$ (если число подгрупп = 4) и последующего определения подгрупповых параметров для интервала путем решения системы алгебраических уравнений

$$\langle \sigma_t^n \rangle = \sum_{k=1}^{p} a_k \sigma_k^n \qquad (p = 2,3 \; ; \; n = \pm 1, \pm 2, \pm 3 - 4),$$

$$\langle \sigma_k \sigma_t^n \rangle = \sum_{k=1}^{p} a_k \sigma_{ik} \sigma_k^n \qquad (p = 2,3 \; ; \; n = 0, +1,2)$$

г) целые положительные числа, большие 3 , резервируются для других возможных способов вычисления подгрупповых характеристик для интервалов.

У. 1. E .
2. Число подгрупп.
3. a_1
4. σ_1

В случае необходимости информация переходит в последующие позиции этой и следующей за ней карт в формате позиций 3-4 карты У.

Этот формат, вообще говоря, позволяет задавать разное число подгрупп для различных E. На практике однако число подгрупп для всех E в пределах данного Δ E обычно одно и тоже.

5) Сечение зависит от энергии. Энергетическая зависимость подгрупповых параметров.

IУ. 1. НТП = 122.
2. Число подгрупп.
3. Число карт для этого НТП .
4. Резерв.
5. Число ИНТ , определяющее закон интерполяции по энергии.
6. Условное число, определяющее способ получения интервальных (групповых) подгрупповых параметров (см. поз.6 карты IУ для НТП = 121).

У. 1. Номер подгруппы (i).
2. Число значений E .
3. Резерв.
4. E_1.
5. a_{i1}
6. σ_{i1}

В случае необходимости информация переходит на последующие карты в формате позиций 4-6 карты У.

Формат карт для НТП с $n_1 = 2$ в настоящее время не определен.

II.2.3. Формат карт для представления данных о параметрах разрешенных резонансов

а. Общая информация

I. 1. НТП.
2. Резерв.
3. Число карт для данного НТП.
4-6 Резерв.

II. 1. $E_н$.
2. $E_в$.
3. Число изотопов.
4-6. Резерв.

б. Информация об изотопе

III. 1. Атомный вес I-го изотопа.
2. Его процентное содержание.
3. Число карт для этого изотопа (включая данную).
4. $\pm$ -радиус нейтронного канала (в ферми) (со знаком минус, если задается энергетическая зависимость радиуса или его зависимость от ℓ и J).
5. $\pm$ I - четность и спин ядра-мишени.
6. Число резонансов данного изотопа, параметры которых приводятся.

IV. 1. Число реакций, для которых даются параметры.
2. НЧК реакции упругого рассеяния = 002.
3. НЧК реакции полного радиационного захвата = 102.
4. НЧК реакции деления, если оно имеется, = 019. Если деления нет, то - нуль.
5. НЧК 4-й реакции, если она есть, или 0.
6. НЧК 5-й реакций, если она есть, или 0.

При необходимости информация переходит на последующие карты в формате пов. 5,6 карты IV.

V. 1. Признак наличия нерезонансного сечения рассеяния, НРР:

НРР = 0 если такого вклада нет;
НРР = I если он задан в ряде энергетических точек;
НРР = 2 если он должен рассчитываться по формулам, на основе средних резонансных параметров;
НРР >2 если он должен рассчитываться на иной основе.

2. Признак характера учета проницаемостей и факторов сдвига для нейтронного канала, ХУПН

ХУПН = 0 если эти факторы рассчитываются обычным путем;
ХУПН = 1 если они заданы при фиксированных энергиях;
ХУПН = 2 если они должны рассчитываться по тем или иным формулам.

3. Признак наличия нерезонансного сечения радиационного захвата (аналогично соответствующему признаку для рассеяния), НРЗ.

4. Признак характера учета проницаемостей и факторов сдвига для радиационного захвата, ХУПЗ

ХУПЗ = 0, если эти величины не зависят от энергии (как обычно);

ХУПЗ = − 1, если они даны при фиксированных энергиях вне зависимости от ℓ.

ХУПЗ = + 1, если они даны при фиксированных энергиях для разных ℓ.

ХУПЗ $\geqslant$ 2, если они должны рассчитываться по формулам.

5. Признак наличия нерезонансного сечения деления (аналогично соответствующему признаку для рассеяния, НРД.

6. Признак характера учета проницаемостей и факторов сдвига для деления (аналогично соответствующему признаку для захвата), ХУПД. Если кроме упругого рассеяния, захвата и деления имеются и другие реакции, информация о наличии для них нерезонансного вклада и о характере учета проницаемостей и факторов сдвига записывается на последующих картах в формате позиции 3–4 карты У.

в. Задание радиусов нейтронных каналов

УI.
1. Максимальное значение ℓ, для которого задаются $a_{\ell y}$.
2. Нуль, если радиусы нейтронных каналов проводятся вне при фиксированных энергиях.
   Единица, если величины $a_{\ell y}(E)$ должны рассчитываться по средним резонансным параметрам пропущенных уровней.

УП.
1. Первое значение ℓ.
2. Число энергий, при которых задаются $a_{\ell y}$ для данного ℓ.
3. Число значений y, для которых задаются $a_{\ell y}$ для данного ℓ.
4. Первое значение y для данного ℓ.
5. Второе значение y для данного ℓ.
6. Третье значение y для данного ℓ и т.д.

Если число значений y для данного ℓ больше 3, то информация переходит на последующие карты в формате поз. 4–6 карты УП.

VIII. 1. E - энергия ($= E_n$ если радиусы задаются при одной энергии)
2. $a_{\ell y}(E)$ для данного ℓ и первого значения y.
3. $a_{\ell y}(E)$ для данного ℓ и второго значения y и т.д. (с переходом на последующие карты если число значений y больше 5).

Карты типа VII, VIII и IX повторяются для $\ell = 1, 2, \ldots, \ell_{max}$.

г. Задание нерезонансных сечений

(если хотя бы одно из них задается в виде таблицы сечений при фиксированных энергиях).

IX. 1. НЧК для первой реакции, для которой задается нерезонансное сечение.
2. Число энергетических точек.
3. Число карт с данными для этого нерезонансного сечения (включая данную).
4-6. Резерв.

X. 1. E_1.
2. σ_1, и т.д.

При необходимости информация переходит на последующие карты в формате карты XI. Карты типа X и XI повторяются для каждой реакции, для которой задается нерезонансное сечение.

д. Задание проницаемостей и факторов сдвига

(если хотя бы одной реакции проницаемости и факторы сдвига задаются в виде таблиц при фиксированных энергиях)

XI. 1. НЧК = 02.
2. Число ℓ, для которых задаются энергетические зависимости проницаемостей и т.п.
3. Число карт с данными о проницаемостях и факторах сдвига для рассматриваемой реакции.
4. Признак зависимости данных от $\ell (= 1)$.
5-6. Резерв

XII. 1. ℓ_1.
2. Число энергетических точек для данного ℓ ($= \ell_1$)
3. Число карт с данными о проницаемости и факторах сдвига для данного ℓ.
4-5. Резерв.

XIII. 1. E_1.
2. $P_{\ell_1}(E_1)$.
3. $\delta_{\ell_1}(E_1)$.
4. E_2.
5. $P_{\ell_1}(E_2)$.
6. $\delta_{1\ell}(E_2)$.

Информация переходит на последующие карты в формате карты XIII. Карты типа XIII и XIV повторяются для всех нужных ℓ.

Проницаемости для остальных реакций, не характеризующихся орбитальным моментом вылетающей частицы.

XIV. 1. НЧК соответствующей реакции.
2. Число энергетических точек.
3. Число карт с данными о проницаемостях и факторах сдвига для рассматриваемой реакции.
4. Признак независимости данных от $\ell (= -1)$.
5-6. Резерв.

XV. 1. E_1.
2. $P_n(E_1)$.
3. $\delta_n(E_1)$.
4. E_2.
5. $P_n(E_2)$.
6. $\delta_n(E_2)$.

Информация переходит на последующие карты в формате карты XV.

Карты типа XII-XIII или XIV -XV повторяются для всех реакций, для которых задаются энергетические зависимости проницаемостей факторов сдвига. При этом проницаемости для реакций, характеризующихся орбитальным моментом вылетающей частицы, задаются в формате карт XII -XIII, где вместо ℓ пробивается ℓ'.

а) Собственно резонансные параметры

XVI. 1. E_r - резонансная энергия I-го резонанса.
2. $\pm J$ - четность и спин составного состояния.
3. $\pm \ell$ - наименьший орбитальный угловой момент нейтронов, которые могут образовывать указанное состояние. Набивается со знаком минус, если состояние может образовываться и нейтронами с большим орбитальным моментом.
4. Γ_{rn} $(|E_r|)$ - нейтронная ширина.
5. $\Gamma_{r\gamma}$ - радиационная ширина [x].
6. Γ_{rf} - делительная ширина [xx].

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x) Если проницаемость для какой-либо реакции зависит от энергии, ширина задается при энергии $|E_r|$.

xx) Более 4-х входных ℓ форматок не предусматривается.

Если $\ell < 0$, то следующая карта имеет вид:

XVII. 1. $\pm \ell_2$ - следующий угловой момент нейтронов, которые могут образовывать данное состояние (со знаком минус, если он не максимальный из возможных).
2. $\Gamma_{rn\ell_2}(|E_r|)$ - соответствующая нейтронная ширина.
3. $\pm \ell_3$ (если $\ell_2 < 0$). В противном случае в позициях 3 ÷ 6 набиваются нули.
4. $\Gamma_{rn\ell_3}$ $(|E_r|)$
5. ℓ_4 *) (если $\ell_3 < 0$). В противном случае в позициях 5 ÷ 6 набиваются нули.
6. $\Gamma_{rn\ell_4}$ $(|E_r|)$

Если есть реакции, отличные от $(n,n),(n,\gamma),(n,f)$, то

XVIII 1. НЧК для первой из таких реакций.
2. $\Gamma_{r\alpha_1}(|E_r|)$ - соответствующая ширина при $E=|E_r|$
3. ℓ' - орбитальный момент вылетающей частицы.
4. НЧК для второй из таких реакций
5. $\Gamma_{r\alpha_2}(|E_r|)$ - соответствующая ширина для $E=|E_r|$
6. ℓ' - орбитальный момент вылетающей частицы.

При необходимости информация переходит на последующие карты в формате карты XVII.

Карты типа XVI - XVII повторяются для каждого резонанса в порядке возрастания E_r.

Карты типа II-XVII повторяются для каждого изотопа.

II. 2.4. Формат карт для представления данных о статистических параметрах неразрешенных резонансов (НОК = 01, n_1 = 4)

а) Общая информация

I. 1. НТП.
2. Резерв.
3. Число карт для этого НТП.
4-6. Резерв.

II. 1. $E_н$ - нижняя граница области, в которой рекомендуется проведение расчетов по параметрам неразрешенных резонансов.
2 $E_в$ - верхняя граница этой области.
3. Резерв.
4. Число изотопов.
5. Условное число $\varkappa p$, определяющее характер изменения средних резонансных параметров:
$\varkappa p$ = 1, если эти параметры постоянны в интервале,
$\varkappa p$ = 2, если они линейно меняются от одной энергетической точки к другой,
$\varkappa p$ = 3, если они считаются постоянными в пределах подинтервалов, на которые разбивается интервал.

6. Число энергетических точек (если $xp = 2$) или подинтервалов (если $xp = 3$) или нуль (если $xp = 1$).

б) Информация об изотопе

III. 1. Атомный вес первого изотопа.
2. Его процентное содержание.
3. Число карт с данными об этом изотопе.
4. Радиус нейтронного канала в ферми (пробивается со знаком минус, если задается его энергетическая зависимость и (или) зависимость от ℓ и J).
5. $\pm$ 1 - четность и спин ядра-мишени.
6. Резерв.

IV. 1. Число реакций, для которых даются параметры.
2. НЧК реакции упругого рассеяния = 002.
3. НЧК реакции полного радиационного захвата = 102.
4. НЧК реакции деления = 019 (если оно имеется) или 0.
5. НЧК 4-й реакции, если она есть, или 0.
6. НЧК 5-й реакции, если она есть, или 0.

При необходимости информация переходит на следующие карты типа IV.

V. 1. Признак наличия нерезонансного сечения рассеяния $Нрр$
$Нрр = 0$, если такого вклада нет
$Нрр = 1$, если он задан при дискретных энергиях или в подинтервалах вместе со средними резонансными параметрами.
$Нрр > 1$, если он должен рассчитываться по тем или иным формулам.
2. Признак характера учета проницаемостей и факторов сдвига для нейтронного канала, $хупн$.
$хупн \pm 0$, если эти проницаемости рассчитываются обычным путем.
$хупн = 1$, если они заданы при дискретных энергиях или в подинтервалах вместе со средними резонансными параметрами.
$хупн > 1$, если они должны рассчитываться тем или иным формулам.

3. Признаки наличия нерезонансного сечения радиационного захвата, $Нрэ$ (аналогично соответствующему признаку для рассеяния).
4. Признак характера учета проницаемостей и факторов сдвига для радиационного захвата, $хупэ$:
$хупэ = 0$, если эти величины не зависят от энергии (как обычно),
$хупэ = -1$, если даны вместе со средними резонансными параметрами при фиксированных энергиях или в подинтервалах вне зависимости от ℓ .
$хупэ = +1$, если они даны вместе со средними резонансными параметрами для разных ℓ .
$хупэ > 1$, если они должны рассчитываться по тем или иным формулам.

5. Признак наличия нерезонансного сечения деления (аналогично соответствующему признаку для рассеяния), Нрд.
6. Признак характера учета проницаемостей и реакторов сдвига для деления (аналогично соответствующему признаку для захвата), Хупд. Если кроме упругого рассеяния, захвата и деления имеются и другие реакции, информация о наличии для них нерезонансного вклада и о характере учета проницаемостей и факторов сдвига записывается на последующих картах в формате поз. 3–4 карты У.

в) Информация для энергетической точки или интервала

УI. I. E : если Хр = I, то $E = E_в$;
если Хр = 2, то E – это энергетическая точка, при которой задаются средние резонансные параметры (первая точка должна совпадать с $E_н$, а последняя с $E_в$);
если Хр = 3, то E есть верхняя энергетическая граница подинтервала (для последнего подинтервала она должна совпадать с $E_в$).
2. Та четность составного ядра, которая рассматривается первой (+ I или –I). Если здесь 0, то данные не зависят от четности состояния составного ядра.
3. Число карт для данной энергетической точки (подинтервала), включая данную карту.
4. Число рассматриваемых значений J – спинов составного ядра.
5–6. Резерв.

Задание радиусов нейтронных каналов

(если радиус a в поз. 4 карты II отрицателен)

УП. I. $l_м$ – максимальное значение l для которого задаются a_{cJ}
2. Резерв.
3. Число карт с информацией о радиусе, включая данную
4–6. Резерв.

УШ. I. Первое значение $l = l_m$ (наименьшее).
2. Число значений J, для которых задаются a_{cJ} для данного l.
3. Первое (наименьшее) значение J.
4. Следующее значение J и т.д.

При необходимости информация о значениях J переходит на следующую карту в формате поз. 3–6 карты УШ.

IX. I. a_{cJ} для данного l и первого значения J
2. a_{cJ} для данного l и следующего значения J и т.д. с переходом по последующие карты, если число значений J более 6.

Карты типа УШ и IX повторяются для $l = l_{m+1}, l_{m+2}, \ldots, l_м$.

Задание нерезонансных сечений реакций (если хотя бы для одной из них, согласно данным карты У (поз. 1,3,5) и однотипных с ней карт, таковой вклад имеется).

X. 1. Число реакций, для которых приводятся нерезонансные вклады.
2. Резерв.
3. Число карт с информацией о нерезонансных вкладах в сечения.
4-6. Резерв.

XI. 1. НЧК 1-й реакции, для которой проводится нерезонансный вклад.
2. Соответствующий вклад в сечение .
3. НЧК 2-й реакции с нерезонансным вкладом в сечение.
4. Соответствующий вклад
и т.д. с переходом на последующие карты в том же формате.

Задание проницаемостей и факторов сдвига

(если хотя бы для одной реакции согласно данным карты У (поз. 2,4,6) и однотипных с ней карт, предусмотрено задание проницаемостей и факторов сдвига)

XII. 1. Число реакций, для которых даются проницаемости и факторы сдвига.
2. Резерв.
3. Число карт с информацией о проницаемостях и факторах сдвига.
4-6. Резерв.

XIII. 1. НЧК 1-й реакции, для которой приводятся проницаемости и факторы сдвига.
2. Проницаемость для 1-реакции.
3. Фактор сдвига уровня 1-й реакции.
4. НЧК 2-й реакции, для которой приводятся проницаемости и факторы сдвига.
5. Проницаемость для 2-й реакции .
6. Фактор сдвига для 2-й реакции.

При необходимости информация переходит на последующие карты в формате карты XIII.

7. Информация для определенного спинового состояния

IX. 1. J - спин составного ядра (начиная с наименьшего).
2. N - число возможных значений ℓ для данных J, π и E[x])

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x) Шаг изменения ℓ , $\delta\ell = (\ell_{max} - \ell_{min}) / (N-1)$. Если возможно лишь упругое рассеяние, то $\delta\ell = 2$. Если есть неупругое рассеяние, то возможно и $\delta\ell = 1$.

3. Число карт с информацией для данного набора J, π, E.
4. l_{min} - наименьшее значение l для данных J, π, E.
5. l_{max} - наибольшее значение l для данных J, π, E.
6. $D_{J\pi}$ - среднее распределение между уровнями для данных J, π, E.

X. 1. Средняя радиационная ширина, $\bar{\Gamma}_{\gamma, J\pi}$.
2. Число степеней свободы для $\bar{\Gamma}_{\gamma, J\pi}$
3. Средняя делительная ширина, $\bar{\Gamma}_{f, J\pi}$
4. Число степеней свободы для $\bar{\Gamma}_{f, J\pi}$
5. Средняя приведенная нейтронная ширина для $l = l_{min}$, $\bar{\Gamma}_n^{(0)}, J, l_{min}$.
6. Число степеней свободы для $\bar{\Gamma}_{n, J, l_{min}}^{(0)}$.

Если $l_{max} \neq l_{min}$, то данные о $\bar{\Gamma}_{n, J, l}^{(0)}$ и соответствующих числах степеней свободы набиваются на последующих картах в формате поз. 5 и 6. карты XI.

XI. Данные для реакций, отличных от упругого рассеяния, полного радиационного захвата и деления (если таковые реакции входят в перечень, указанный в карте IУ или последующих картах типа IУ).

1. НЧК данной реакции.
2. Число значений l', возможных при этой реакции (= I, если реакция не характеризуется орбитальным моментом вторичных нейтронов).
3. Первое значение l' (если в поз. 2 стоит единице, эта информация не используется).
4. Средняя приведенная ширина для данной реакции и рассматриваемого значения l'.
5. Число степеней свободы для этой реакции при рассматриваемом значении l'. Если приведенная ширина канала данной реакции принимается не флуктуирующей, число степеней свободы условно полагается равным нулю.
6. Резерв.

Если число допустимых значений l' больше одного, информация переходит на последующие карты в формате поз. 3,4 и 5 карты XI.

Карты IX - XI повторяются для каждого значения J и π при данной энергии (или для данного энергетического интервала).

Карты УI - XI повторяются для каждой энергии (или энергетического интервала).

Карты II - XI повторяются для каждого изотопа.

3. Угловые распределения вторичных частиц (НОК = 02)

Угловое распределение вторичных частиц $f(\theta)$, представляющее собой нормированное распределение вероятности рассеяния

$$f(\theta) = \frac{\int d\varphi\, \sigma(\theta,\varphi)}{\int d\varphi \int d\theta\, \sigma(\theta,\varphi)}$$

может задаваться как для некоторого энергетического интервала в целом, так и в его отдельных энергетических точках. Предполагается, что имеет место следующее условие нормировки:

$$\int_0^{\pi} f(\theta) \sin\theta\, d\theta = 1.$$

Предусматривается задание угловых распределений в дискретных точках по μ, где $\mu = \cos\theta$, θ – угол рассеяния (μ – представление) и параметрически путем задания коэффициентов ω_ℓ разложения $f(\theta)$ в ряд по полиномам Лежандра $P_\ell(\cos\theta)$ (ω – представление)

$$f(\theta) = \frac{1}{2}\left[1 + \sum_{\ell=1}^{n} \omega_\ell P_\ell(\cos\theta)\right]$$

Значения μ задаются в порядке их возрастания от – I до + I. Угол θ может быть взят как в системе центра масс, так и в лабораторной системе координат. Сведения о системе отсчета указываются в дополнительной информации заголовка НТП специальным условным числом co:

условное число системы отсчета $\begin{cases} co=1 & \text{– данные в системе центра масс,} \\ co=2 & \text{– данные в лабораторной системе.} \end{cases}$

Использование той или иной системы отсчета зависит от вида реакции. В случае процессов упругого рассеяния и неупругого рассеяния с возбуждением отдельных уровней ядра, когда существует простая связь между энергиями первичных и вторичных частиц, по-видимому, целесообразно выбрать систему центра масс. Для прочих неупругих процессов данные обычно задаются в лабораторной системе. При этом необходимо иметь в виду следующее. В тех случаях, когда имеется простое аналитическое выражение, связывающее энерго-угловые распределения в этих двух системах координат, в принципе безразлично в какой системе будут приведены данные в библиотеке. Если же такая связь между системами для данной реакции отсутствует, произвольно выбирать систему координат нельзя. Решающую роль здесь начинают играть факторы наличия данных в той или другой системе, требования практики и возможности обрабатывающих программ.

Выбор значений E и μ в случае μ-представления должен обеспечивать достаточную точность получения вероятности для любой энергии и угла рассеяния с помощью интерполирования между имеющимися в библиотеке величинами. В случае ω-представления необходимая точность обеспечивается заданием достаточного числа коэффициентов разложения (число n).

Несмотря на то, что угловое распределение задается нормированной функцией вероятности, в тех случаях, когда истинное угловое распределение в μ -представлении аппроксимируется приближенно, например, линейными отрезками, результирующее представление, вообще говоря, уже не будет нормированным. На практике поэтому в некоторых случаях может потребоваться дополнительная нормировка угловых распределений, полученных из библиотечных данных.

Форматы предусматривают возможность задания полного углового распределения $f(\theta)$ в виде линейной комбинации некоторого числа частичных распределений $f_i(\theta)$, взятых с определенными весами a_i:

$$f(\theta) = \sum_{i=1}^{k} a_i f_i(\theta)$$

Отдельные $f_i(\theta)$ могут описывать, например, различные угловые распределения продуктов некоторого ядерного процесса, который протекает разными путями и поэтому описывается с помощью разных механизмов. Указанная возможность позволяет также использовать для описания резонансной структуры угловых распределений подгрупповое представление. В этом случае a_i имеют смысл долей подгрупп, а $f_i(\theta)$ характеризует угловое распределение данной подгруппы нейтронов.

Принятые в настоящее время форматы требуют, чтобы все входящие в сумму $f_i(\theta)$ были заданы в одном и том же представлении (либо в μ -представлении, либо в ω - представлении) и относились к одной и той же системе координат. Структура НТП позволяет, однако, в случае необходимости избавиться от этого ограничения.

Во всех случаях полная область энергии, в которой рассматриваются угловые распределения, должна совпадать с энергетической областью задания соответствующих интегральных сечений. Если, допустим, сечение упругого рассеяния задается в области от 0,001 эв до 14 Мэв, тогда в точечном по энергии представлении первое угловое распределение должно быть дано при энергии 0,001 эв и последнее - при 14 Мэв; для интервального представления нижняя граница первого интервала должна быть 0,001 эв, а верхняя граница последнего интервала - 14 Мэв. Это обстоятельство может облегчить выявление грубых ошибок в задаваемых данных.

3.1. Классификация НТП для НОК = 02

Способ задания данных по угловым распределениям определяется старшим разрядом НТП в соответствии со следующей таблицей.

n	Способ задания угловых распределений
1	В дискретных точках по μ (μ - представление).
2	Параметрически путем задания коэффициентов разложения в ряд по полиномам Лежандра (ω -представление).

Последующие значения n_1 (3-9) резервируются для новых способов, если таковые будут появляться.

Два младших разряда НТП для $n_1 = 1$ и $n_1 = 2$ имеют следующий смысл:

n_2 – означает число переменных или параметров, от которых могут зависеть угловые распределения,

n_3 – определяет порядок старшинства этих параметров относительно друг друга.

Для двух переменных (энергия E и вероятность углового распределения или доля подгруппы a_i) идентификация младших разрядов НТП определяется таблицей

$n_2 n_3$	Старшая переменная	Младшая переменная
01	–	–
02	–	–
11	E	–
12	a_i	–
21	E	a_i
22	a_i	E

3.2. Формат карт для НОК = 02

I. 1. НТР.
2. Число Δ E для этого НТР.
3 A – атомный вес
4–6. Резерв.

II. 1. $E_н$.
2. $E_в$.
3. Число карт для этого Δ E, включая данную.
4. Число групп вторичных частиц для которых задаются угловые распределения в этом ΔE .
5–6. Резерв.

III. 1. Условное число, отождествляющее группу вторичных частиц.
2. Число НТП угловых распределений для этой группы частиц.
3. Число карт для представления угловых распределений этой группы, включая данную карту.
4.
5. } Резервируются для дополнительной информации об этой группе
6. вторичных частиц.

Формат следующих карт зависит от НТП.

I) Угловое распределение изотропно в ΔE.

В этом случае на карте IУ указывается лишь номер типа представления (НТП = 101 для μ-представления, НТП = 201 для ω-представления) и условное число системы отсчета.

IУ.	1. НТП = 101.	IУ. 1. НТП = 201.
	2. Условное число системы отсчета, со.	2. Условное число системы отсчета, $\Delta\Phi$.

2) Угловое распределение для всего ΔE.

IУ.	1. НТП = 102.	IУ. 1. НТП = 202.
	2. Условное число системы отсчета, со	2. Условное число системы отсчета, со.
	3. Число значений μ	3. Число значений ω
	4. Число ИНТ, определяющее закон интерполяции $f(\mu)$ по μ.	4. ω_1
	5. μ_1	5. ω_2
	6. $f(\omega_1)$	6. ω_3

3) Угловые распределения при фиксированных E.

IУ.	1. НТП = 111.	IУ. 1. НТП = 211.
	2. Число значений E.	2. Число значений E.
	3. Число карт для этого НТП.	3. Число карт для этого НТП.
	4. Условное число системы отсчета, со.	4. Условное число системы отсчета, со.
	5. Число ИНТ, определяющее законы интерполяции по E и по μ	5. Число ИНТ, определяющее закон интерполяции ω_ℓ по E.
	6. Число значений ∂,M, если оно общее для всего ΔE, или нуль.	6. Число значений ω, если оно общее для всего ΔE, или нуль.
У.	1. E.	У. 1. E.
	2. Число значений μ	2. Число значений ω.
	3. μ_1	3. ω_1
	4. $f(\mu_1)$ и т. д.	4. ω_2 и т.д.

4) Суперпозиция угловых распределений для всего ΔE.

IУ.	1. НТП = 112.	IУ. 1. НТП = 212.
	2. Число значений α.	2. Число значений α.
	3. Число карт для этого НТП.	3. Число карт для этого НТП.

4. Условное число системы отсчета, с о.
5. Число ИНТ, определяющее закон интерполяции $f(\mu)$ по μ
6. Резерв.

4. Условное число системы отсчета, с о.
5,6. Резерв.

У. I. a.
2. Число значений μ
3. μ_1
4. $f(\mu_1)$ и т. д.

У. I. a
2. Число значений ω
3. ω_1
4. ω_2 и т. д.

5) Суперпозиция угловых распределений при фиксированных энергиях E.

IУ. I. НТП = 121.
2. Число значений E.
3. Число карт для этого НТП.
4. Условное число системы отсчета, с о.
5. Число ИНТ, определяющее законы интерполяции $a(E)$ по E, $f(E,\mu)$ по E и $f(E,\mu)$ по μ.
6. Число значений μ, если оно общее для всего ΔE, или нуль

IУ. I. НТП = 221.
2. Число значений E.
3. Число карт для этого НТП.
4. Условное число системы отсчета, с о.
5. Число ИНТ, определяющее законы интерполяции $a(E)$ по E и $\omega_E(E)$ по E.
6. Число значений ω, если оно общее для всего ΔE, или нуль.

У. I. E.
2. Число значений a.
3. Число карт для этого E.
4,5. Резерв.
6. Число значений μ, если оно общее для всех a или нуль.

I. E.
2. Число значений a.
3. Число карт для этого E.
4,5. Резерв.
6. Число значений ω, если оно общее для всех a, или нуль.

УI. I. a.
2. Число значений μ для этого a.
3. μ_1
4. $f(\mu_1)$ и т.д.

I. a.
2. Число значений ω для этого a.
3. ω_1
4. ω_2 и т.д.

6) Угловые распределения с данным a при различных значениях E

IУ. I. НТП = 122.
2. Число значений a.
3. Число карт для этого НТП

IУ. I. НТП = 222.
2. Число значений.
3. Число карт для этого НТП.

4. Условное число системы отсчета, со.
5. Число ИНТ, определяющее законы интерполяции $a(E)$ по E, $f(E,\mu)$ по E и $f(E,\mu)$ по μ.
6. Число значений E, если оно общее для всех a, или нуль.

4. Условное число системы отсчета, со.
5. Число ИНТ, определяющие законы интерполяции $a(E)$ по E и $w_E(E)$ по E.
6. Число значений E, если оно общее для всех a, или нуль.

У. 1. a.
2. Число значений E.
3. Число карт для этого a.
4-5. Резерв.
6. Число значений μ, если оно общее для всех E, или нуль.

У. 1. a.
2. Число значений E.
3. Число карт для этого a.
4-5. Резерв.
6. Число значений w, если оно общее для всех E, или нуль.

УI. 1. E.
2. Число значений μ.
3. μ_1
4. $f(\mu_1)$ и т.д.

УI. 1. E.
2. Число значений w
3. w_1
4. w_2 и т.д.

Во всех рассмотренных здесь НТП для иллюстрации форматов позиций, непосредственно занятых под данные по угловым распределениям, приведен минимальный объем информации: одна пара (μ, $f(\mu)$), одно значение w. Предполагается, что в случае необходимости эта информация переходит в последующие позиции той же самой карты или следующих за ней карт в указанных выше форматах.

4. Энергетические распределения вторичных частиц (НОК = 03)

Когда известна аналитическая зависимость между энергиями первичных и вторичных частиц, нет необходимости задавать энергетическое распределение вторичных частиц; оно легко может быть подсчитано с помощью специальных программ обработки данных. В противном случае должен быть указан закон распределения вторичных частиц по энергиям.

В настоящее время предусматривается задание информации по энергетическим распределениям в формате следующих законов.

Закон 1. Испускание частиц с известной дискретной энергией (например, вылет запаздывающих нейтронов деления).

Закон 2. Испускание частиц с энергией $E = k\,(E_0 - E_d)$, где E_0 - начальная энергия, E_d - некоторое дискретное значение энергии, K - константа (коэффициент ослабления). Неупругое рассеяние нейтронов с возбуждением отдельных уровней ядра входит сюда как частный случай; при этом K учитывает среднюю передачу энергии ядру отдачи.

Закон 3. Независящий от начальной энергии непрерывный нормированный спектр нейтронов деления вида

$$S(E) = A\, e^{-BE} \operatorname{sh} \sqrt{cE}$$

где A,B,C - некоторые постоянные.

Закон 4. Спектр нейтронов деления, учитывающий зависимость от начальной энергии нейтрона и свойств делящегося ядра, задается нормированной функцией вероятности

$$N(E) = \alpha \frac{E}{T^2} \exp\left(-\frac{E}{T}\right) + (1-\alpha)\left(\frac{2}{\pi^{1/2}} B^{3/2}\right) E^{1/2} \exp\left(-\frac{E}{B}\right)$$

где

$$B = a + b\,(\bar{\nu}+1)^{1/2}$$

$$\alpha = (\sigma_{n,n'f} + \sigma_{n,2nf}) / \bar{\nu}\,(\sigma_{nf} + \sigma_{n,n'f} + \sigma_{n,2nf}),$$

$$T = c\,(E_0 - E_f)/(14 - E_f)$$

Здесь a, b, c - константы; $\bar{\nu}$ - среднее число нейтронов деления, E_f - порог реакции $(n, n'f)$, E_0 - начальная энергия, σ_{nf}, $\sigma_{n,n'f}$ и $\sigma_{n,2nf}$ - сечения реакций (n, f), $(n, n'f)$ и $(n, 2nf)$. Этот закон полностью определяется заданием четырех параметров: a, b, c, E_f (остальные величины могут быть взяты из массивов библиотеки).

Закон 5,6,7. Спектр вылетающих частиц описывается нормированной функцией вероятности следующего вида:

$$f(E_0, E) = p(E/E_0^q),$$

где E_0 - начальная энергия, E - энергия вылетающих частиц. Параметр q принимает значения

$$q = \begin{cases} 0 & \text{для закона 5,} \\ I/2 & \text{для закона 6,} \\ I & \text{для закона 7} \end{cases}$$

Закон 6 включает в себя спектр испарения.

Закон 8. Спектр вылетающих частиц задается произвольной функцией начальной (E_0) и конечной (E) энергий в дискретных точках (если нет зависимости от E_0, этот закон будет совпадать с законом 5).

Для законов 5-7 данные по энергетическим распределениям задаются парами величин (аргумент $x = E/E_0^q$, соответствующая ему вероятность $p(x)$ с таким расчетом, чтобы любые промежуточные значения величин в хорошем приближении могли быть получены интерполированием соседних, хранящихся в библиотеке, значений. Следует заметить, что хотя функции вероятностей в случае законов 5-7 нормированы внутри области задания аргументов (с определенной степенью точности), может случиться, что некоторые значения аргу-

ментов будут недоступны на практике в силу закона сохранения энергии (например, может оказаться, что при заданном значении аргумента энергия вторичной частицы будет больше начальной энергии). В таких случаях, как правило, будет необходима дополнительная перенормировка функции распределения вероятности.

Также как и в случае угловых распределений, формат представления энергетических распределений вторичных частиц предусматривает задание результирующих распределений в виде суперпозиции некоторого числа законов с их вероятностями. Каждый закон в этом случае отвечает одному из возможных механизмов протекания ядерного процесса. Указанную возможность здесь также можно интерпретировать как подгрупповое представление энергетических распределений вторичных частиц; при этом вероятности законов будут играть роль долей подгрупп, а сами законы характеризовать энергетические распределения для соответствующих подгрупп нейтронов.

Особый случай рассеяния нейтронов при тепловых энергиях будет рассмотрен отдельно.

4.1. Классификация НТП для НОК = 03

Способ задания данных по энергетическим распределениям вторичных частиц определяется старшим разрядом НТП в соответствии со следующей таблицей.

n_1	Способ задания энергетических распределений
I	В формате законов, когда начальная энергия явно не задается.
2	В форме законов, когда начальная энергия задается явно.

Последующие значения n_1 (3-9) резервируются для других способов задания, если таковые будут появляться.

Два младших разряда НТП имеют следующий смысл:

$n_2 n_3 = 01 \div 49$ - резервируются для задания распределения одним законом и означают номер соответствующего закона,

$n_2 n_3 \geqslant 50$ - резервируются для задания распределения суперпозицией законов в следующих случаях:

$n_2 n_3 = 50$ - явно не задано E_0 ;

$n_2 n_3 = 51$ - все законы при данном E_0 ;

$n_2 n_3 = 52$ - все E_0 для данного закона.

4.2. Формат карт для НОК = 03

I. I. НТР.
2. Число ΔE для этого НТР.
3-6. Резерв.

II. 1. $E_н$.
2. $E_в$.
3. Число карт для этого ΔE, включая данную.
4. Число групп вторичных частиц, для которых задаются энергетические распределения в этом ΔE.
5,6. Резерв.

III. 1. Условное число группы вторичных частиц.
2. Число НТП энергетических распределений этой группы частиц.
3. Число карт для представления энергетического распределения этой группы, включая данную карту.
4-6. Резерв.

Формат последующих карт зависит от НТП.

1) закон 1.

IУ. 1. НТП = 101.
2. Число значений дискретных энергий E_n, с которыми испускаются частицы.
3. Значение E_n
4. Соответствующая вероятность $p(E_n)$

2) закон 2.

IУ. 1. НТП = 102.
2. Число рассматриваемых пар (E_d, k).
3. Резерв.
4. E_d.
5. k.
6. Соответствующее значение вероятности p.

3) закон 3 и 4.

IУ. 1. НТП = 103.
2. A
3. B
4. C
5. }
6. } Нули

IУ. 1. НТП = 104
2. a
3. b
4. c
5. E_f
6. Нуль

4) законы 5,6,7

IУ. 1. НТП = 105 (106 или 107).
2. Число точек спектра.
3. Резерв.
4. Число ИНТ, определяющее закон интерполяции $p(x)$ по x.
5. Первое значение $x = E/E_0$.
6. Соответствующая ему вероятность $p(x)$.

5) Линейная комбинация законов (E_* явно не задано)

IУ. 1. НТП = I50
2. Число различных законов в линейной комбинации.
3. Число карт для этого НТП.
4-6. Резерв.

Формат карты У зависит от номера закона и имеет вид:

а) Для законов I и 2.

У. 1. Номер закона = 0I.
2. Вероятность этого закона.
3. Число дискретных E_n.
4.
5. } Резерв.
6.

У. 1. Номер закона = 02.
2. Вероятность этого закона.
3. Число пар (E_d, k)
4. E_d
5. k
6. Значение ρ.

б) Для законов 3 и 4.

У. 1. Номер закона = 03.
2. Вероятность этого закона.
3. A
4. B
5. C
6. Нуль

У. 1. Номер закона = 04.
2. Вероятность этого закона.
3. a
4. b
5. c
6. E_+

в) для законов 5 (6,7)

У. 1. Номер закона = 05 (06 или 07)
2. Вероятность данного закона
3. Число точек спектра
4. Число ИНТ , определяющее закон интерполяции $\rho(x)$ по x.
5. x.
6. $\rho(x)$.

6) закон 8.

IУ. 1. НТП = 208.
2. Число значений E_* .
3. Число карт для этого НТП.
4. Число ИНТ , определяющее законы интерполяции $\rho(E_*, E)$ по E_* и $\rho(E_*, E)$ по E.
5,6. Резерв

У. 1. E_*.
2. Число значений E при этом E_*.
3. E.
4. $\rho(E)$.

7) Линейная комбинация законов (все законы при данном E_0)

IV. 1. НТП = 251.
2. Число значений E_0.
3. Число карт для этого НТП.
4. Число ИНТ, определяющее закон интерполяции вероятности закона по начальной энергии E_0.
5,6. Резерв.

V. 1. E_0
2. Число законов при этом E_0.
3. Число карт для этого E_0.
4-6. Резерв.

Формат последующих карт зависит от номера закона и имеет вид:

а) Для закона 8.

VI. 1. Номер закона = 08.
2. Вероятность этого закона.
3. Число значений E.
4. Число ИНТ, определяющее закон интерполяции $p(E)$ по E.
5. E.
6. $p(E)$.

б) для законов 1-7 формат карты VI НТП = 251 совпадает с форматом карты V НТП = 150.

8) Линейная комбинация законов (все E_0 для данного закона)

IV. 1. НТП = 252
2. Число различных законов.
3. Число карт для этого НТП.
4-6. Резерв.

V. 1. Номер закона
2. Число значений E_0.
3. Число карт для этого закона.
4. Вероятность этого закона
5. Число ИНТ, определяющее закон интерполяции вероятности закона по начальной энергии E_0, и, если требуется, закон интерполяции $p(E_0, E)$ по E_0 и $p(E_0, E)$ по E.
6. Резерв.

Формат последующих карт зависит от номера закона и имеет вид:

а) Для закона 1

VI. 1. E_0.
2. Число дискретных E_n.
3. E_1.

б) Для закона 2

VI. 1. E_0.
2. Число пар (E_d, p)
3. Резерв

4. $p(E_1)$.
5. E_2
6. $p(E_2)$ и т.д.

в) Для закона 3

УI. I. E_0.
2. A.
3. B.
4. C.
5,6. Нули.

д) Для законов 5 (6,7)

УI. I. E_0.
2. Число точек спектра
3. x_1
4. $p(x_1)$
5. x_2
6. $p(x_2)$ и т.д.

4. E_d.
5. K.
6. p.

г) Для закона 4

УI. I. E_0.
2. a.
3. b.
4. c.
5. E_1
6. Нуль.

УI. I. E_0
2. Число значений E при этом E_0
3. E_1
4. $p(E_1)$
5. E_2
6. $p(E_2)$ и т.д.

5. Энерго-угловые распределения тепловых нейтронов (НОК = 04)

Данные по энерго-угловым распределениям рассеяния тепловых нейтронов характеризуют взаимодействие нейтронов с атомными ядрами в области энергий, где необходимо принимать во внимание относительное движение нейтронов и ядра и взаимодействие атомов (эффекты химической связи и т.п.) Такого рода информация может быть задана различными способами. В настоящее время форматами предусматривается представление энерго-угловых распределений тепловых нейтронов в виде матрицы двойных дифференциальных сечений и в форме закона рассеяния.

В первом случае задается матрица числовых значений функции $\sigma(E_0 \to E, \Theta)$, представляющей собой вероятность для нейтрона, имеющего начальную энергию E_0, рассеяться на угол Θ и иметь после рассеяния энергию E. Дискретные значения переменных (E_0, E, Θ), от которых зависит функция вероятности рассеяния тепловых нейтронов, выбираются с таким расчетом, чтобы любые требуемые значения функции могли быть с хорошей точностью получены с помощью интерполяции содержащихся в матрице величин.

В том случае, когда энерго-угловое распределение тепловых нейтронов определяется законом рассеяния, задается матрица значений $S(\alpha, \beta)$ при дискретных значениях переменных.

$$\alpha = [E_0 + E - 2(E_0 E)^{1/2} \cos\theta] / A'kT$$

и

$$\beta = (E - E_0)/kT$$

Здесь E_0 – начальная энергия нейтронов, E – конечная энергия, θ – угол рассеяния в лабораторной системе, kT – температура в энергетических единицах, A' – отношение массы ядра к массе нейтрона (это определение можно распространить и на случай молекул). Параметры α и β, таким образом, связаны с передачей импульса и энергии в результате столкновения. Выбор значений переменных α и β должен обеспечивать возможность получения с достаточной степенью точности любых значений $S(\alpha, \beta)$ методом интерполирования.

Выражение для сечения процесса, в результате которого нейтрон с начальной энергией E_0 рассеется на угол θ в лабораторной системе координат и будет обладать энергией E, имеет вид

$$\sigma(E_0 \to E, \theta) dE d\cos\theta = \frac{\sigma_b}{kT} \sqrt{\frac{E}{E_0}} \exp(-\beta/2)\, S(\alpha,\beta)\, dE\, d\cos\theta$$

Здесь σ_b – сечение для связанного атома

$$\sigma_b = \sigma_{fr} \left(\frac{A+1}{A}\right)^2$$

σ_{fr} – сечение для свободного атома.

Для одноатомного газа, когда эффекты химической связи не играют роли, функция рассеяния $S(\alpha,\beta)$ определяется выражением

$$S(\alpha,\beta) = \frac{1}{2\sqrt{\pi\alpha}} \exp[-(\alpha^2+\beta^2)/4\alpha]$$

Приближение газовой модели часто используется для задания функции $S(\alpha,\beta)$ в тех случаях, когда отсутствует другая информация по закону рассеяния тепловых нейтронов.

Когда $S(\alpha,\beta)$ имеет особенность при $\beta = 0$ в виде δ-функции, ее можно представить следующим образом

$$S(\alpha,\beta) = S^*(\alpha,\beta) + e^{-\lambda\alpha}\delta(\beta)$$

В этом случае место $S(\alpha,\beta)$ в библиотеке занимает $S^*(\alpha,\beta)$, а величина λ задается на картах заголовка НТП в виде дополнительной информации. Здесь же задаются:

σ_{fr} – сечение для свободного атома, если оно постоянно,
$\mathcal{E} = E_{гр}/kT$ – величина, отвечающая нижней границе справедливости статической модели упругого рассеяния,

E_m - верхняя граница постоянства σ_{fr} ; выше этого значения необходимо учитывать энергетическую зависимость сечения σ_{fr} , полагая его равным, например, имеющемуся в библиотеке сечению упругого рассеяния (НТР = 01002) и пренебрегая вкладом неупругого рассеяния из-за его малости.

A' - эффективное отношение масс атома (молекулы) к массе нейтронов; для молекул эта величина в известной мере условна и обычно выбирается исходя из анализа экспериментальных результатов.

5.1. Классификация НТП для НОК = 04

Способ задания данных по энерго-угловым распределениям тепловых нейтронов определяется старшим разрядом НТП в соответствии со следующей таблицей:

n_1	Способ задания энерго-угловых распределений
1	В виде матрицы вероятностей рассеяния
2	В виде матрицы функции рассеяния $S(\alpha,\beta)$

Два младших разряда НТП определяют порядковый номер формата при данном значении n_1 .

5.2. Формат карт для НОК = 04

I. 1. НТР.
2. Число рассматриваемых температур.
3. Резерв.
4. Число ИНТ , определяющее закон интерполяции $\sigma(E_0,E,\theta,T)$ или $S(\alpha,\beta,T)$ по температуре Т.

II. 1. Температура, которой соответствуют данные.
2. Число НТП при этой температуре.
3. Число карт для этой температуры, включая настоящую карту.
4-6. Резерв

Формат следующих карт зависит от НТП.

I) НТП = 100

III. 1. НТП = 100.
2. Число значений E_0 .
3. Число карт для этого НТП.
4. Число ИНТ , определяющее законы интерполяции $\sigma(E_0,E,\theta)$ по E_0 , по E и по θ.
5,6. Резерв.

IУ. 1. E_0.
2. Число значений E при этом E_0.
3. Число карт для этого E_0.
4–6. Резерв.

У. 1. E.
2. Число значений θ при этом E.
3. Θ.
4. $\sigma(\Theta)$.

2) НТП = 200

У. 1. НТП = 200.
2. Число значений β.
3. Число карт для этого НТП.
4. λ.
5. σ_{fr}.
6. ε.

IУ. 1. E_m.
2. A'
3. Резерв.
4. Число ИНТ, определяющее законы интерполяции $S(\alpha,\beta)$ по β и по α.
5,6. Резерв

У. 1. β.
2. Число значений α при этом β
3. α_i
4. $S(\alpha_i)$ и т.д.

6. Специальные величины для нейтронов – $\bar{\nu}$, α, η и т.д. (НСК = 05)

К таким величинам относятся:

h – число вторичных нейтронов на столкновение (упругое и неупругое)

$$h = (\sigma_n + \sigma_{n'} + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu}\sigma_f + \dots) / \sigma_t .$$

η – число вторичных нейтронов на неупругое столкновение

$$\eta = (\sigma_{n'} + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu}\sigma_f + \dots) / \sigma_x .$$

α – отношение сечения захвата к сечению деления

$$\alpha = \sigma_\gamma / \sigma_f$$

$\bar{\nu}$ – среднее число вторичных нейтронов на деление.

В дальнейшем может возникнуть необходимость в определении аналогичных величин для некоторых других данных.

Три первых величины являются производными величинами и поэтому могут быть вычислены по соответствующим формулам; задание их в библиотеке в этом случае не обязательно. Напротив, $\bar{\nu}$ измеряется непосредственно в эксперименте и должно быть задано для всех делящихся изотопов ядер.

Способы представления специальных нейтронных величин аналогичны способам представления сечений. Поэтому сохраняют силу все указания, сделанные при обсуждении формата для НОК = 01. Обратим внимание лишь на следующее обстоятельство. Величины $\bar{\nu}$ могут задаваться в точках, не совпадающих с точками задания других сечений, в частности, сечений деления. Поэтому следует требовать, чтобы совпали самые крайние (наименьшая и наибольшая) энергетические точки, в которых заданы $\bar{\nu}$ и σ_f. В этом случае можно будет находить значения $\bar{\nu}$ и σ_f, необходимые для вычисления величин $\bar{\nu}\sigma_f$, путем интерполирования.

6.1. Классификация НТП для НОК = 05

Классификация НТП для специальных нейтронных величин аналогична соответствующей классификации для нейтронных сечений (НОК = 01).

6.2. Формат карт для НОК = 05

Формат карт для представления специальных нейтронных величин совпадает с форматом представления нейтронных сечений (НОК = 01), за исключением того, что в позиции 5 карты I для НОК = 05 ничего не пробивается.

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ПЛАНИРОВАНИЕ ОПТИМАЛЬНОЙ СОВОКУПНОСТИ МИКРОСКОПИЧЕСКИХ ЭКСПЕРИМЕНТОВ И ОЦЕНОК ОБЕСПЕЧИВАЮЩЕЙ ЗАДАННУЮ ТОЧНОСТЬ РАСЧЕТА РЕАКТОРНЫХ ПАРАМЕТРОВ

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А Н Н О Т А Ц И Я

Изучается вопрос о потребностях в точности микроскопических ядерных данных, обеспечивающих заданную точность расчета реакторных параметров. В этой связи развит общий метод учета корреляций погрешностей микроскопических величин, относящихся к различным процессам, различным энергетическим группам и различным изотопам. Погрешность рассматривается состоящей из компонент, отличающихся одна от другой корреляционными свойствами. Благодаря такому разбиению и получаются простые формулы для связи этих компонент погрешностей с требуемой точностью реакторного параметра.

Далее использованы методы "планирования экспериментов" для математической формулировки задачи о наименее дорогой совокупности экспериментов обеспечивающих заданную точность расчета реакторного параметра. Решение задачи получено в виде простых формул.

Вычислены требования на все компоненты погрешности. Показана возможность смягчить требования при измерении потока нейтронов одним и тем же методом в экспериментах по σ_f и σ_c.

Показывается особая важность погрешности в нормировке кривой и подчеркивается особая роль оценки в определении этой погрешности.

I. ВВЕДЕНИЕ

а) Вариация реакторного параметра как функция вариаций микроскопических (групповых) величин

Расчетное значение каждого реакторного параметра "с", например эффективного коэффициента размножения, коэффициента воспроизводства КВ и т.п., зависит от большого числа различных микроскопических величин таких как

эффективные сечения взаимодействия при разных энергиях нейтронов, числа вторичных нейтронов деления и т.д. Обычно расчеты делаются в рамках групповой модели. Относительные вариации групповых величин $\left(\frac{\delta\sigma}{\sigma}\right)_{\alpha ij}$, соответствующих величине типа " α " изотопа " i " в группе j определяют относительную вариацию реакторного параметра $\delta C/C$ через линейное соотношение

$$\delta C/C = \sum_{\alpha ij} S_{\alpha ij}\left(\frac{\delta\sigma}{\sigma}\right)_{\alpha ij} \qquad (1)$$

Коэффициенты этого соотношения $S_{\alpha ij}$ называемые коэффициентами чувствительности, вычисляются с помощью обобщенной теории возмущений [1]

б) Постановка и решение задачи об определении необходимых точностей ядерных констант в предшествующих работах

Для определения погрешности в реакторном параметре "C" надо сделать предположение о том, как складываются вклады от многих погрешностей входящих в формулу (I). Если принять, что эти вклады являются случайными величинами, некоррелированными между собой, то, в соответствии с правилами математической статистики, дисперсия или иначе квадрат стандартного отклонения реакторного параметра "C" - D^2 ($D^2 \equiv \overline{(\delta C/C)^2}$) выражается через дисперсии групповых микроскопических величин $d^2_{\alpha ij}$ ($d^2_{\alpha ij} \equiv \overline{(\delta\sigma/\sigma)^2_{\alpha ij}}$) следующим образом:

$$D^2 = \sum_{\alpha ij} S^2_{\alpha ij}\, d^2_{\alpha ij} \qquad (2)$$

Такое предположение было использовано в работе Мурхэда [2], который вычислял коэффициенты чувствительности прямым расчетом в пяти-групповой модели. Граблер, Хатчинс и Лимфорд [3] поставили вопрос о важности в рассматриваемой задаче учета корреляции в погрешностях. Они высказали мнение, что реально почти каждой ядерной константе можно сопоставить 2-3 корреляционных интервала на всей энергетической оси. Здесь можно отметить, что в работе [2] фактически использовано 5 корреляционных интервалов, т.к. использован 5-ти групповой расчет.

Зарицкий и Троянов [4] провели очень подробное исследование рассматриваемого вопроса, рассчитали широкий класс быстрых реакторов с использованием обобщенной теории возмущений в 18-ти групповой модели и провели сравнительные исследования необходимой точности констант для всех этих реакторов. Авторы выписали также формулы для необходимых точностей констант, приводящих к заданной точности реакторного параметра как для некоррелированных констант, так и для констант скоррелированных в пределах некоторых интервалов. При этом для распределения требований по погрешности различных величин в правой части формулы (2) потребовали одинаковый вклад от разных источников погрешностей, т.е. наложено требование:

$$d_{\alpha ij} = \frac{const}{|S_{\alpha ij}|} \qquad (3)$$

В последней работе Зарицкого, Николаева, Троянова [5] обосновано требование на 1% точность в $K_{эфф}$ и 2% точность в КВ. Выработаны также требования на точность измерений большого круга микроскопических величин на основе предположения о статистической независимости погрешности в каждой из 18 групп. При этом произведено некоторое отступление от принципа равного вклада различных констант (3), исходя из интуитивных соображений о сравнительной достижимости точностей различных констант, что делалось методом подбора и последовательных приближений.

В этой работе особый интерес представляет мысль о выработке требований на точности отношений величин к стандартам таким как $\bar{\nu}$ Cf-252 и сечение деления урана-235, а также на точность самих стандартов. Такие требования выработаны, но на основе того же предположения о некоррелированности ошибок в 18 группах.

в) Критика предшествующих работ и необходимость корректного подхода к анализу структуры погрешностей

Сопоставление результатов описанных выше работ [2-5] показывает, что при определении необходимой точности существенное влияние на ее величину оказывает предположение о коррелированность или некоррелированности ошибок. В работе [3] это влияние оценивается фактором 3-5. Более того в зависимости от учета корреляции [2,3,4] или неучета их [5] требования на точность микроконстант меняются от невыполнимых в обозримое время до почти уже выполненных.

Поскольку решение этого вопроса существенно влияет на определение научной политики, представляется необходимым развить более корректный подход к анализу корреляций погрешностей и в целом к решению задачи о планировании совокупности микроскопических экспериментов.

Основным недостатком всех указанных работ, устранению которого посвящена данная работа, с нашей точки зрения является то, что погрешность каждой величины рассматривалась как целое не имеющей структуры и считалась либо целиком скоррелированной с погрешностями соседних величин либо целиком нескоррелированной. Но при более внимательном рассмотрении становится ясным, что надо учитывать структуру погрешности, отдельные компоненты которой отличаются одна от другой корреляционными свойствами.

2. КОМПОНЕНТЫ ОТНОСИТЕЛЬНОЙ ПОГРЕШНОСТИ ГРУППОВОЙ МИКРОСКОПИЧЕСКОЙ ВЕЛИЧИНЫ И ИХ СВЯЗЬ С ПОГРЕШНОСТЬЮ РЕАКТОРНОГО ПАРАМЕТРА

а) Обозначения и понятия

Относительная погрешность групповой микроскопической величины входящая в соотношение (I) обозначена ниже $(\delta\%_\sigma)_{ij}$

Индексы:

i - номер изотопа

j - номер группы

α - характеризует величину и принимает значения, определяемые таблицей:

Величина	Индекс вместо α
Среднее число вторичных нейтронов деления	$\bar{\nu}$
Сечение деления	f
Сечение радиационного захвата	c
Доля спектра деления в группу "к"	$\chi_к$
Сечение перехода в группу "К"	$пер_к$
Транспортное сечение	tr

Погрешность, определяемая из микроскопического эксперимента величины характеризуется стандартным отклонением " $d_{\alpha ij}$ ", вероятностный смысл которого определяется формулой:

$$d^2_{\alpha ij} = \overline{\left(\delta\sigma/\sigma\right)^2_{\alpha ij}} \qquad (4)$$

где $\left(\delta\sigma/\sigma\right)_{\alpha ij}$ рассматривается как случайная величина, а черта означает усреднение по большому числу измерений. Однако определенное в соответствии с(4), т.е. по разбросу экспериментальных значений в конкретном опыте, стандартное отклонение является лишь статистической компонентой погрешности. Дело в том, что в опыте обычно производится привязка к некоторому стандарту. Поэтому действительная погрешность должна включать в себя наряду со статистической систематическую погрешность метода привязки или в нашей терминологии - погрешность нормировки, а также погрешность самого стандарта. Смысл введенного в формулу (5) вектора f_j будет пояснен ниже. Таким образом:

$$\left(\delta\sigma/\sigma\right)_{\alpha ij} = \left(\delta\sigma/\sigma\right)^{стат}_{\alpha ij} + \left(\delta\sigma/\sigma\right)^{норм}_{\alpha i} f_j + \left(\delta\sigma/\sigma\right)^{станд} \qquad (5)$$

Обычно при вычислении полной ошибки опыта все три указанные компоненты погрешности считаются некоррелированными между собой и складываются квадраты стандартных отклонений, связанные с $\left(\delta\sigma/\sigma\right)$ формулой (4)

$$d^2_{\alpha ij} = \left(d^{стат}_{\alpha ij}\right)^2 + \left(d^{норм}_{\alpha i}\right)^2 f^2_j + \left(d^{станд}\right)^2 \qquad (6)$$

При этом статистический смысл $d^{стат}_{\alpha ij}$ и $d^{станд}$ ясен. $d^{стат}_{\alpha ij}$ определяется в самом рассматриваемом опыте, а $d^{станд}$ берется из паспорт-

ных данных стандарта или стандартной методики. Что же касается смысла $d_{ij}^{норм}$, то он появляется лишь при рассмотрении некоторой мыслимой совокупности экспериментов, проводимых разными методами, по которым в соответствии с определением (4) можно провести усреднение. Отсюда ясно, что оценить из опыта погрешности привязки или нормировки кривой можно только на основе анализа нескольких независимых по методам экспериментов, т.е. в процессе оценки ядерных данных.

б) Корреляционные свойства компонент погрешности

Рассмотрим каждый из трех членов правой части соотношения (5). Первый член имеет чисто статистическую природу и некоррелирован ни с другими энергетическими группами, ни с другими типами процессов, ни с другими изотопами. Если в пределах одной группы имеется n экспериментальных точек со статистической ошибкой каждой из них d, то

$$d_{ij}^{стат} = d/\sqrt{n} \qquad (7)$$

Соотношение (7) надо иметь в виду при рассуждениях о величине допустимой статистической ошибки.

Третий член постоянен для всех тех групп, веществ и типов величин, при измерении которых применяется рассматриваемый стандарт. Таким образом, эта компонента погрешности полностью скоррелирована в области применения стандарта. Укажем на два примера. Если при измерениях среднего числа вторичных нейтронов используется калибровка по калифорнию, то $(\delta\sigma/\sigma)^{станд.}$ является погрешностью в значении $\bar{\nu}$ калифорния 252. Если рассмотреть совокупность измерений различных сечений, в которых поток нейтронов измеряется одним и тем же способом, то под $(\delta\sigma/\sigma)^{станд.}$ следует понимать систематическую ошибку данного метода измерения потока.

Второй член представляет компоненту погрешности, скоррелированную в различных энергетических группах, т.е. ошибку в нормировке кривой. При измерениях сечений эта компонента погрешности может проистекать, например, от ошибки в определении количества исследуемого вещества в слое, от систематической ошибки при детектировании событий, соответствующих измеряемой величине, от ошибки в измерении абсолютного потока нейтронов, или в эталонном сечении, по которому определялся поток нейтронов, если эта ошибка не учитывается в третьем члене.

При измерениях $\bar{\nu}$ по калифорниевому стандарту рассматриваемая компонента погрешности может проистекать, в частности, от различия в жесткостях спектров деления $Cf\text{-}252$ и исследуемого изотопа, которое может привести к различию в эффективностях регистрации нейтронов.

При наличии нескольких независимых погрешностей с одинаковыми корреляционными свойствами их можно объединить по обычному правилу квадратичного сложения.

Иногда возможно ввести расчетную поправку на систематическую погрешность. Тогда погрешностью в нормировке остается погрешность этой поправки. В подобных случаях мы можем сделать заключение о ходе этой погрешности с номером группы.

Для описания этого хода введем вектор f_j, равный единице в группе с максимальной ошибкой, нулю или отрицательной величине в тех группах, где рассматриваемая систематическая ошибка из физических соображений должна обратиться в нуль или изменить знак.

Необходимо отметить, что сечения и потоки нейтронов в разных областях энергии измеряются разными методами. Поэтому в качестве одного из вариантов следует выбрать соответственно этим областям и корреляционные интервалы, в каждом из которых справедливо соотношение (5), а между собой они не скоррелированы.

в) Корреляция погрешностей оцененных данных

Оценка данных должна производиться с учетом корреляционных свойств погрешностей экспериментальных данных. В частности, например, ошибка в нормировке кривой сечения при наличии нескольких экспериментальных работ должна быть определена из их совокупности. Таким образом, в процессе оценки эта ошибка определяется, а не исчезает, как это, по существу, предполагается в работе [5]. Поэтому при выработке требований к точности оцененных, рекомендованных данных следует учитывать корреляционные свойства погрешностей, описанные выше.

г) Погрешности в реакторном параметре в зависимости от компонент погрешностей микровеличин

Из сказанного выше ясно, что если по формуле (6) из компонент погрешностей образовать единые погрешности $\delta_{\alpha ij}$, то они оказались бы частично скоррелированными. Поэтому переход от формулы (I) к формуле (2) не является корректным.

В данной работе предлагается естественный путь преодоления этой трудности. А именно, в соотношение обобщенной теории возмущений (I) представляется покомпонентное представление погрешности (5) и группируются члены с одинаковыми $\delta\sigma/\sigma$.

$$\frac{\delta C}{C} = \sum_{\alpha ij} S_{\alpha ij}\left(\frac{\delta\sigma}{\sigma}\right)^{\text{стат}}_{\alpha ij} + \sum_{\alpha i}\left(\sum_j f_j S_{\alpha ij}\right)\left(\frac{\delta\sigma}{\sigma}\right)^{\text{норм}}_{\alpha i} + \left(\sum_{ij} S_{\nu ij}\right)\left(\frac{\delta\sigma}{\sigma}\right)^{\text{станд}}_{\nu} + \sum_{ij}\left(S_{fij} + S_{cij}\right)\left(\frac{\delta\sigma}{\sigma}\right)^{\text{отн.}}_{\text{неопр.}}$$

Первый и второй члены получены без конкретных предположений, третий – в предположении измерений $\bar{\nu}$ всех делящихся изотопов во всей области энергий по калифорниевому стандарту, четвертый – в предположении единого метода измерений потока при измерениях сечений радиационного захвата и деления всех изотопов, по которым подразумевается суммирование по индексу i. В полученном соотношении уже каждая относительная погрешность некоррелирована с другими. Если предположить существование m корреляционных интервалов, о которых сказано в последнем абзаце раздела б), то второй и четвертый члены правой части должны быть разбиты на соответствующие части с независимыми относительными погрешностями

$$\sum_{\alpha i}\Big(\sum_{j} f_j S_{\alpha i j}\Big)\Big(\frac{\delta\sigma}{\sigma}\Big)^{\text{корр}}_{\alpha i} \rightarrow \sum_{\alpha i}\sum_{k=1}^{m}\Big(\sum_{j=n_k}^{m_k} f_j S_{\alpha i j}\Big)\Big(\frac{\delta\sigma}{\sigma}\Big)^{\text{корр}}_{\alpha i}; \sum_{ij}\big(S_{fij}+S_{cij}\big)\Big(\frac{\delta\sigma}{\sigma}\Big)^{\text{стат+корр}}_{\text{потом.}} \rightarrow \sum_{k=1}^{m}\sum_{i}\sum_{j=n_k}^{m_k}\big(S_{fij}+S_{cij}\big)\Big(\frac{\delta\sigma}{\sigma}\Big)^{\text{стат+корр}}_{\text{потом.}}$$

n_k и m_k номера первой и последней групп K -го корреляционного интервала. Правую часть полученного соотношения перепишем в виде одинарной суммы от единицы до N , где N – число независимых погрешностей $^{\ell}(\delta\sigma/\sigma)$. Левый верхний индекс ℓ принимает значения от I до N . Коэффициент перед $^{\ell}(\delta\sigma/\sigma)$ обозначим Z_ℓ . Очевидно, что

$$Z_\ell = \begin{cases} S_{\alpha i j} \\ \sum_{j=n_k}^{m_k} f_j S_{\alpha i j} \\ \sum_{i}\sum_{j=1}^{m} S_{\alpha i j} \\ \sum_{i}\sum_{j=n_k}^{m_k}\big(S_{fij}+S_{cij}\big) \end{cases} \qquad k=1,\dots m \tag{8}$$

$$\delta C/C = \sum_{\ell=1}^{N} Z_\ell\, {}^{\ell}(\delta\sigma/\sigma) \tag{9}$$

Поскольку все $^{\ell}(\delta\sigma/\sigma)$ случайные некоррелированные величины, получаем для дисперсии реакторного параметра выражение через дисперсии соответствующих величин:

$$D^2 = \sum_{\ell=1}^{N} Z_\ell^2\, d_\ell^2 \tag{10}$$

где $D^2 \equiv \overline{(\delta C/C)^2}$ $d_\ell^2 \equiv \overline{{}^{\ell}(\delta\sigma/\sigma)^2}$ (см. раздел 2а)

В соотношении (10) учет коррелированности компонент погрешностей выражается в том, что коэффициенты перед отдельными средними квадратичными ошибками оказываются квадратами сумм коэффициентов чувствительности.

3. МИНИМИЗАЦИЯ ЗАТРАТ НА СОВОКУПНОСТЬ МИКРОСКОПИЧЕСКИХ ЭКСПЕРИМЕНТОВ И ОЦЕНОК, НЕОБХОДИМЫХ ДЛЯ ДОСТИЖЕНИЯ ЗАДАННОЙ ТОЧНОСТИ РЕАКТОРНЫХ РАСЧЕТОВ

а) Теория и формулы

В этом разделе мы будем пользоваться понятием статистического веса эксперимента или совокупности экспериментов, равного обратной величине среднеквадратичной ошибки

$$w_\ell = 1/d_\ell^2 \tag{11}$$

Стоимость ℓ -го эксперимента считается, как это часто делается в "планировании эксперимента", пропорциональной статвесу и равной $\lambda_\ell w_\ell$ где λ_ℓ -константа, имеющая смысл стоимости получения единицы статвеса при определении ℓ -ой величины.

Соответственно этому общая стоимость системы экспериментов по измерению микроскопических констант, обеспечивающих заданную точность расчета реакторного параметра, складывается из стоимостей каждого из необходимых экспериментов, а также совокупностей экспериментов.

$$\text{Общая стоимость} = \sum_{\ell=1}^{N} \lambda_\ell w_\ell \qquad (12)$$

Мы заинтересованы в достижении минимальными затратами заданной точности реакторного параметра δ_0^2 , которая также выражается через статвеса, если в (10) подставить (11)

$$\delta_0^2 = D^2 = \sum_{\ell=1}^{N} Z_\ell^2 / w_\ell = \sum_{\ell=1}^{N} Z_\ell^2 d_\ell^2 \qquad (13)$$

Задача на минимум выражения (12) при дополнительном условии (13) решается известным методом неопределенных множителей Лагранжа, в котором ищется экстремум выражения

$$B = \sum_{\ell=1}^{N} \lambda_\ell w_\ell + \lambda \sum_{\ell=1}^{N} Z_\ell / w_\ell$$

где λ - неопределенный множитель Лагранжа.

Приравнивая частные производные по w_ℓ нулю, получаем систему N уравнений $\frac{\partial B}{\partial w_\ell} = 0$; $\lambda_\ell - \lambda \frac{Z_\ell^2}{w_\ell^2} = 0$; $\frac{1}{\lambda} = \frac{Z_\ell^2}{w_\ell^2 \lambda_\ell} = \frac{Z_\ell^2 d_\ell^4}{\lambda_\ell}$

Исключая $1/\lambda$, получаем $N - 1$ уравнений

$$d_\ell / d_k = \left(Z_k / Z_\ell\right)^{1/2} \left(\lambda_\ell / \lambda_k\right)^{1/4} \qquad (14)$$

Пользуясь этим соотношением и выражая d_ℓ через d_1 в соотношении (13), которое является N -ным по счету, записываем:

$$\delta_0^2 = d_1^2 Z_1^2 + d_1^2 \left(\frac{Z_1}{Z_2}\right)\left(\frac{\lambda_2}{\lambda_1}\right)^{1/2} Z_2^2 + \cdots + d_1^2 \left(\frac{Z_1}{Z_N}\right)\left(\frac{\lambda_N}{\lambda_1}\right)^{1/2} Z_N^2$$

Из последнего соотношения определяем d_1 , а из соотношения (14) точности d_ℓ всех остальных экспериментов.

На случай если вычисленные погрешности некоторых величин оказываются большими чем их значения, предположенные достигнутыми, в программе расчета следует предусмотреть блок со следующими функциями. Выявляются все такие члены, вычисляется их вклад в общую погрешность по формуле $\sum Z_\ell^2 d_\ell^2$ этот вклад вычитается из δ_0^2 и после этого вся процедура проводится снова для оставшихся членов. Следует предусмотреть возможность итераций

до полной сходимости этого процесса. Таким образом находятся требуемые точности всех входящих в расчет величин, достижение которых обеспечивает выполнение требования к точности расчета реакторного параметра при минимальных затратах.

б) Определение относительной стоимости экспериментов на основе гипотезы о равной "пробивной способности" экспериментаторов

Для определения относительной стоимости экспериментов, т.е. отношений $\lambda_e/\lambda_к$ мы предположили, что для получения статвесов во всех экспериментах, выполненных к настоящему времени было затрачено одинаковое количество средств. Иными словами мы предполагали, что разными измерениями в среднем по разным институтам и странам, занимались экспериментаторы с равной способностью "пробивать" средства на эксперимент и различие в достигнутой точности характеризует сравнительные объективные трудности проведения экспериментов. Таким образом:

$$\lambda_e W_e = \lambda_к W_к$$

Задавая достигнутые к настоящему времени W_e, $W_к$ мы получаем отношения: $\lambda_e/\lambda_к = W_к/W_e = d_e^2/d_к^2$

Можно было бы ввести к "коэффициент внимания" к величине "К" - КВВк для определения $\lambda_e/\lambda_к$ использовать $\frac{\lambda_e W_e}{КВ_e} = \frac{\lambda_к W_к}{КВ_к}$

в) Расчитанные требуемые точности

Коэффициенты чувствительности взяты для реактора на окиси плутония-239 и урана-238 объемом 5 тыс. литров из работы [4].

Принятые нами для определения сравнительной стоимости экспериментов предположения о достигнутой точности приведены в таблице. Приведены результаты, соответствующие $K_{эфф} = \pm 0{,}01$. Эти точности обеспечивают и КВ = ± 0,02.

г) Обсуждение результатов

Предположение о чисто статистической природе ошибок приводит к существенной недооценке необходимых точностей эксперимента. В этом предположении достигнутая точность уже удовлетворяет требованиям.

Введение в рассмотрение возможности ошибок в нормировке кривых т.е. систематических ошибок, сразу делает требования очень жесткими и трудно выполнимыми в ближайшее время, особенно, имея ввиду точность 0,7% в σ_f плутония и 1,7% в сечении захвата урана-238. При разбиении всей области энергии на три корреляционных интервала $E_1 > 1{,}4$ Мэв $> E_2 > 0{,}1$ Мэв $> E_3$ указанные требования несколько смягчаются до 1,1% в σ_f плутония и до 2,4% в σ_c урана-238.

Таблица

Величина	Предположение о достигнутой точности %		Сумма $\sum Z^2 \times 10^4$, определяющая средние по энергии допустимые погрешности			Вклад систематической погрешности и погрешности стандарта в δ_*^2	Погрешность в %, обеспечивающие $K_{эфф} = \pm 1\%$ усредненные по всей области энергий, определенные по формуле $d = \sqrt{вклад / \sum Z^2}$ * *					
	Статистическая компоненты погрешности	Погрешность в нормировке или в стандарте	12 несколлированных групп	Погрешность скоррелированная во всей области энергий	3 корреляционных интервала		Чисто статистическая погрешность %	Погрешность скоррелированная по всей области		Реалистический вариант 3 корреляц. интервала		
								Поток в каждом опыте измеряется независимо	Единый метод измерения потока $d_{норм.}$ или $d_{станд.}$	Поток в каждом опыте измеряется независимо	Единый метод измерения потока $d_{норм.}$ или $d_{станд.}$	$\sqrt{d_{норм.}^2 + d_{станд.}^2}$
Сечение деления Pu^{239}	1	2	390	3850	1690	0,138	2,6	0,75	0,6	1,1	0,9	2,2
Сечение деления U^{238}	1	2	28	66,5	66,5	0,018	5,5	2,0	1,6	2,0	1,6	2,6
Сечение захвата Pu^{239}	2	10	3,8	31,2	21,5	0,062	17	5,5	4,4	6,7	5,4	5,7
Сечение захвата U^{238}	2	5	88	758	426	0,152	5,7	1,7	1,4	2,1	1,9	2,8
$\bar{\nu}$ Pu^{239}	0,5	1	750	7450	7450	0,096	1,6	0,36	0,36	0,36	0,36	0,5
$\bar{\nu}$ U^{238}	0,5	1	700	180	180	0,015	2	0,91	0,91	0,91	0,91	1
$\bar{\nu}$ Cf^{252}	-	1	-	10000	10000	0,112	-	0,33	0,33	0,33	0,33	-
Поток нейтронов	-	5	-	1400	507	0,208	-	-	1,2	-	2,0	-

ПРИМЕЧАНИЯ: x) В вариантах не чисто статистических из $\delta_*^2 = 1$ 0,8 идет на систематические ошибки и ошибки в стандарте., 0,1 идет на статистические ошибки , 0,1 оставлено на вклад погрешностей неучтенных величин.

xx) В вариантах без потоке и калифорниевого стандарта их вклады перераспределяются по другим величинам.

Указанные погрешности включают и погрешности абсолютного измерения потока и погрешности из-за остальных причин, ведущих к систематическому смещению величины.

Измерение потока нейтронов в экспериментах по сечениям захвата и деления единым методом вводит корреляцию погрешностей различных сечений, которая в отличии от корреляции между погрешностями в соседних энергетических группах, заметно ослабляет требования на точность. Так для σ_f Pu^{239} теперь требуется точность для двух обсуждаемых вариантов соответственно вместе с потоком 1,45% и 2,2%, а для σ_c U^{238} – 2,2% и 2,8%.

Мы считаем, что предположение о трех корреляционных интервалах является реалистическим, т.е. наиболее близким из рассмотренных вариантов к реальной экспериментальной ситуации.

Поэтому, именно для этого случая мы сделали следующие расчеты. Во-первых, точность, которая предположена достигнутой дает $K_{эфф} = \pm 1{,}8\%$. Во-вторых, расчет на основе требований к точности работы [5] дает $K_{эфф} = \pm 1{,}5\%$, а не $\pm 1\%$, как это считали авторы работы.

Это показывает, что наши требования на точность в среднем в 1,5 раза более жесткие. Различие не больше по той причине, что в работе [5] хотя и не предполагалось ошибок в нормировке, что эквивалентно некоррелированности погрешностей в различных группах, но скоррелированность ошибок от стандартов Cf^{252} и сечения урана-235 была учтена.

ВЫВОДЫ

Из результатов работы можно сделать следующие выводы. Требования на точность можно уменьшить рациональным выбором корреляции в измерениях. Надо стремиться скоррелировать измерения захвата и деления разных изотопов имея ввиду разные знаки коэффициентов чувствительности. То же самое следует сделать и в процессе оценки ядерных данных. Но и при этом для выполнения этих требований требуется еще очень большая работа. Это прежде всего относится к требованию измерений абсолютного потока нейтронов с точностью 2%, абсолютного значения $\bar{\nu}$ Cf^{252} с точностью 0,33% $\bar{\nu}$ плутония-239 относительно калифорния с точностью в нормировке 0,36%, захвата U^{238} с систематической погрешностью не превышающей 1,9%.

Надо отметить необходимость дальнейшего анализа требуемой точности микроскопических констант на основе развитого выше метода. Надо включить в рассмотрение другие изотопы и другие сечения кроме рассмотренных. В данной работе они учтены резервированием 0,1 из $\delta_c^2 = 1$. Это приблизительно верно, как можно заключить из результатов работы [5].

Из всего рассмотрения следует постановке требований на работы по оценке.

В этих работах должны быть проанализированы все ожидаемые выше компоненты погрешности и даны оценки их величин. Только в этом случае можно определить погрешность расчета реакторного парметра за счет оцениваемой величины и потребность в дальнейшей работе по ее измерениям и оценке.

Наиболее важная погрешность в нормировке кривых может быть объективно определена только в процессе оценки при анализе работ, выполненных разными методами. Определение этой погрешности не менее важно, чем определение средней величины.

В заключение авторы выражают глубокую благодарность М.Ф. Троянову, З.Д.Кузьминовой, Г.Н.Смиренкину, В.А.Толстикову за обсуждение работы и Давлетшину А.Н. за помощь в расчетах.

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ROLE AND EFFICIENCY OF NUCLEAR THEORY IN EVALUATION RESOLVED AND UNRESOLVED RESONANCES

by

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Abstract

In this paper, we briefly examine various topics linked with the theories used to describe or to calculate the neutron cross section in the field of resonances.

The various formalisms utilized have specific fields of application ; comparisons between the results of different formalisms are difficult, and dangerous.

The theories predicting the statistical distributions of partial widths and of level spacings are well known and verified, with some uncertainty on the number of degree of freedom, ν ; but, the existence of correlations is generally not well established. The only one which is certain (between spacing) has probably little importance for reactor physics ; we try to give some figures of the influence of ν and of these correlations on the calculated cross sections in the unresolved energy range.

The problem of the representation of the data in this unresolved energy range is dependent on the variations with energy of the average data, and on the existence of intermediate structures. Several methods can be considered, the probability distributions of cross sections being probably a very convenient one, if reactor physicists can use them.

1. FORMALISMS UTILIZED

In the formalisms currently utilized in low energy nuclear physics, the neutron cross sections are related to a matrix element $U_{n\alpha}$ by the following formulae :

$$\sigma_{n,\alpha} = \pi \lambda^2 \sum g|U_{n\alpha}|^2 \qquad (1.a)$$

$$\sigma_{n,n} = \pi \lambda^2 \sum g|1 - U_{nn}|^2 \qquad (1.b)$$

$$\sigma_{n,t} = \sum \sigma_{n,n} = 2\pi \lambda^2 \sum g\, R(1 - U_{nn}) \qquad (1.c)$$

with :

$$\begin{cases} g = \dfrac{2J+1}{2(2I+1)} & (s = \text{neutron spin} = 1/2) \\ \pi\lambda^2 = \dfrac{651000}{E}\left(\dfrac{A+1}{A}\right)^2 & (\pi\lambda^2 \text{ in barns, E in eV}) \ * \end{cases}$$

where : α denote the channel ; I, J are respectively the spin of the target and compound nuclei ; E is the energy in the laboratory system.

The factor $\left(\frac{A+1}{A}\right)^2$ should not be omitted as it happens frequently**. The sum are over all the possible values of :

J the spin of the compound nucleus

s,s' the channel spins

ℓ,ℓ' the angular momenta

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* The factor 651 000 is based on (Ta 69) :
h = $6.626\,196 \times 10^{-34}$ sec. (relative error = 7.6×10^{-6})
1 eV = $1.602\,1917 \times 10^{-19}$, (relative error = 4.4×10^{-6})
1 amu = $1.660\,531 \times 10^{-27}$ kg (relative error = 6.6×10^{-6})
neutron mass = 1.0086652 amu (relative error = 0.1×10^{-6})

** This factor should be $(\frac{M+1.008665}{M})^2$. Its approximation by $(\frac{A+1}{A})^2$ introduces an error which is maximum for light nuclei. It is worth 8.8×10^{-4} for ^{6}Li, 1.7×10^{-4} for ^{56}Fe and 0.35×10^{-4} for ^{235}U.

The total cross section in equation (1.c) can be expressed as a linear function of $U_{n,n}$ only if U is unitary.

1.1. The "Breit and Wigner" single level formula which dates from 1936 [Br 36] can be deduced from all the known rigorous formalisms in the approximation : $\Gamma << D$. For the total cross section, it consists of the first 3 terms of equations (13) or (16). It is the most widely used formula because it is easy to handle and gives a sufficient accuracy in many cases.

1.2. The "R matrix" formalism has been developed in the years about 1947 by Wigner and Eisenbud [Wi 47]. It has been reviewed in 1958 by Lane and Thomas [La 58] and there have been few evolutions in it since that time. The expressions of the R matrix elements are very simple :

$$R_{\alpha\alpha'} = \sum_{\lambda} \frac{\gamma_{\lambda\alpha}\,\gamma_{\lambda\alpha'}}{E_\lambda - E} \qquad (2)$$

a) Physical meaning of $\gamma_{\lambda\alpha}$ and E_λ : it is necessary to introduce a boundary between an "internal region" and an "external region". This boundary consists of the "channel surfaces", characterized by channel radius a_α. The E_λ are the eigenvalues, solutions of the Schrödinger wave equation in the internal region : $HX_{\lambda JM} = E_{\lambda J}\, X_{\lambda JM}$, where $X_{\lambda JM}$ is the internal eigenfunction. The quantities $\gamma_{\lambda\alpha}$ (reduced width amplitude) and $\delta_{\lambda\alpha}$ (see [La 58]) are respectively proportional to the values of the internal eigenfunction $X_{\lambda JM}$ and of its derivative on the channel surface ; they are related to the boundary condition parameter B_α by :

$$\frac{\delta_{\lambda\alpha}}{\gamma_{\lambda\alpha}} = B_\alpha \quad .$$

The quantities E_λ, $\delta_{\lambda\alpha}$ and $\gamma_{\lambda\alpha}$ are real, energy independent and have a physical meaning, from which the resonance parameter distribution laws may be deduced. But they depend on a_α and B_α which are more or less arbitrary ; the main criticism against the R matrix formalism is the necessity to introduce

these boundary conditions. However it gives automatically the unitarity condition on the U matrix.

b) Formal exact expression of $U_{\alpha\alpha'}$. The matrix U is related to the R matrix by (the notations are those of Lane and Thomas [La 58]) :

$$\begin{aligned} U &= \Omega\, P^{1/2}\, (1-RL^{\circ})^{-1}\, (1-RL^{\circ *})\, P^{-1/2}\, \Omega \\ &= \Omega\, \left[1 + \beta^{1/2}(1-RL^{\circ})^{-1}\, R\, \beta^{1/2}\, W\right] \Omega \end{aligned} \tag{3}$$

It is possible to split the R matrix in two parts :

$$R = R^{\circ} + R'$$

where R° is supposed to contain the contribution of distant levels, and is expected to vary smoothly with energy. It is possible to introduce a level matrix A taking into account the levels which are included in the matrix R'. The inverse of A is defined by :

$$A^{-1}_{\lambda\lambda'} = (E_{\lambda}-E)\, \delta_{\lambda\lambda'} - \frac{i}{2} \sum_{\alpha} \gamma_{\lambda\alpha}\, \gamma_{\lambda\alpha'} \tag{4}$$

and U can be expressed as a function of R° and A :

$$U = \Omega\, \left\{1 + \beta^{1/2}\left[(1-R^{\circ}L^{\circ})^{-1}\, R^{\circ} + \sum_{\lambda\mu} |\alpha_{\lambda}\rangle\, \langle\alpha_{\mu}|A_{\lambda\mu}\right]\, \beta^{1/2}\, W\right\}\, \Omega \tag{5}$$

with :

$$\alpha_{\lambda} = (1-R^{\circ}\, L^{\circ})^{-1}\, \gamma_{\lambda}.$$

It appears that the calculation of U implies the inversion either of $(1-RL^{\circ})^{-1}$, or of A^{-1}, whose elements may vary rapidly with energy ; these inversions are laborious and time consuming.

c) Simplification. All the practical applications of this theory suppose that :

$$R^{\circ}L^{\circ} = R^{\circ}(L-B) = 0. \tag{6}$$

This can be justified by implicit adequat choice of the a_α and B_α boundary conditions at a given energy ; but condition (6) will not be fulfilled at another energy. With this simplification, the equation (5) can be written :

$$U_{\alpha\alpha'} = e^{-i(\phi_\alpha+\phi_{\alpha'})} \left[\delta_{\alpha\alpha'} + i \sum_{\lambda\lambda'} \gamma_{\lambda\alpha} A_{\lambda\lambda'} \gamma_{\lambda'\alpha'}\right] \qquad (7)$$

1.2.1. Exact calculations. It is necessary to perform a matrix inversion, either A^{-1} or $(1-RL^\circ)$.

The first method used by Vogt in 1958 [Vo 58] implies the inversion, at each energy, of the matrix A^{-1} whose order is equal to the number of levels considered - which may be great.

In the second one, known as the "Reich Moore formalism" [Re 58, Mo 60] the order of the matrix to be inverted should be equal to the total number of channels. But it is possible to share the matrix in a similar way to the channel elimination method of Teichmann and Wigner [La 58] ; then by using the simplification resulting from the statistical hypothesis for the radiation widths, the order of the matrix to be inverted is reduced to the number of retained interfering channels. In practice, several codes are running at present with three channels (one for the neutron, two for the fission widths) and the matrix inversion can be easily written.

This second method is now much more used than the first one ; it is provided in the ENDF library [En 70]. These two methods are exact and use the same parameters ; but it is obliged to do numerical Doppler and resolution broadening.

1.2.2. Case of one channel. If there is only scattering, the R matrix reduces to a function :

$$R_J = \sum_\lambda \frac{\gamma_{n\lambda}^2}{E_\lambda - E} \qquad (8)$$

and U can be expressed by :

$$U^J = e^{-2ika} \frac{1+ikaR_J}{1-ikaR_J} \tag{9}$$

then :

$$\sigma_\alpha = \sigma_t = \pi\lambda^2 \sum g_J \left[1 - e^{-2ika} \frac{1+ikaR_J}{1-ikaR_J}\right]^2 \tag{10}$$

1.2.3. Approximate formulation. It is known since many years that the A matrix can be expanded in series [Wi 46, La 58].

$$A = D + DN^{-1} D + DN^{-1} DN^{-1} D + \ldots \tag{11}$$

where matrices D^{-1} and N^{-1} are respectively the diagonal and the non diagonal part of matrix A^{-1}. This expression (11) converges more or less quickly according to the values of :

$$\sum_\lambda \frac{[\Gamma_{\lambda\alpha}^{1/2} \Gamma_{\lambda'\alpha}^{1/2}]}{E_\lambda - E_{\lambda'}}$$

The U matrix can be expressed as a sum over the resonances :

$$U_{\alpha\alpha'} = e^{-i(\phi_\alpha+\phi_{\alpha'})} \left[\delta_{\alpha\alpha'} + i \sum_\lambda \left(\frac{C^1_{\alpha\alpha'}}{E-\varepsilon_\lambda} + \frac{C^2_{\alpha\alpha'}}{(E-\varepsilon_\lambda)^2} + \ldots\right)\right] \tag{12}$$

This matrix is no more unitary if the expansion is truncated.

If one takes only two terms of the expansion (11), there is only one term in the expression of U. The total cross section, for instance, can then be written as :

$$\sigma_t = 4\pi\lambda^2 \sum_{j s \ell} g_j \left\{ \sin^2\phi_\ell + \cos 2\phi_\ell \sum_\lambda \left(\frac{\Gamma_n}{\Gamma}\right)_\lambda \frac{1}{1+X_\lambda^2} + \sin 2\phi_\ell \sum_\lambda \left(\frac{\Gamma_n}{\Gamma}\right) \frac{X_\lambda}{1+X_\lambda^2} \right.$$

$$+ \sum_\lambda \sum_{\lambda' \neq \lambda} \left(\frac{\Gamma_n}{\Gamma}\right)_\lambda^{1/2} \left(\frac{\Gamma_n}{\Gamma}\right)_{\lambda'}^{1/2} \left(\sum_\alpha [\Gamma_{\lambda\alpha}]^{1/2} [\Gamma_{\lambda'\alpha}]^{1/2} \right) \left(\cos 2\phi_\ell \frac{X_\lambda X_{\lambda'} - 1}{(1+X_\lambda^2)(1+X_{\lambda'}^2)} - \right.$$

$$\left. \left. \sin 2\phi_\ell \frac{X_\lambda + X_{\lambda'}}{(1+X_\lambda^2)(1+X_{\lambda'}^2)} \right) \right\} \tag{13}$$

with $X_\lambda = 2 \frac{E-E_\lambda}{\Gamma_\lambda}$.

This expression of σ_t can be written as :

$$\sigma_t = 4\pi\lambda^2 \sum_{js\ell} g_j \left\{ \sin^2 \phi_\ell + \sum_\lambda \left(\frac{\Gamma_n}{\Gamma}\right)_\lambda \frac{C_{1\lambda}}{1+\chi_\lambda^2} + \sum_\lambda \left(\frac{\Gamma_n}{\Gamma}\right)_\lambda \frac{C_{2\lambda}\ \chi_\lambda}{1+\chi_\lambda^2} \right\}$$

where $C_{1\lambda}$ and $C_{2\lambda}$ are energy independent functions of ϕ_ℓ and of the parameters of all the resonances taken into account.

This method, with 4 terms of (11), has been used at Saclay to analyze the ^{235}U data [Kr 70]. It has the inconvenience to be approximate, and then not valid for all the levels. But it may be interesting for reactor physics : it allows a better description of the cross sections with simple formulae, and has been recommended for this purpose in UK. It has the advantage to allow one to calculate Doppler effect and resolution broadening with the well known ψ, ϕ functions.

The "Multilevel Breit and Wigner" or Bethe formulae. These were established in the years 1937. If one retains just the first term of expansion (11), the elements of U can be simply written :

$$U^J_{n,\alpha} = e^{-i(\phi_\alpha+\phi_{\alpha'})} \left[\delta_{n\alpha} - i \sum_\lambda \frac{[\Gamma_{\lambda n}]^{1/2}\ [\Gamma_{\lambda\alpha}]^{1/2}}{E - \varepsilon_\lambda} \right] \qquad (14)$$

with : $\varepsilon_\lambda = E_\lambda + \Delta_\lambda - \frac{i}{2}\gamma_\lambda$.

The partial cross sections are of the form :

$$\sigma_{n,\alpha} \sim \sum_\lambda \frac{\Gamma_{\lambda n}\ \Gamma_{\lambda\alpha}}{(E-\varepsilon_\lambda)^2} \quad \sum_\lambda \sum_{\lambda' \neq \lambda} \frac{[\Gamma_{\lambda n}]^{1/2}\ [\Gamma_{\lambda' n}]^{1/2}\ [\Gamma_{\lambda\alpha}]^{1/2}\ [\Gamma_{\lambda'\alpha}]^{1/2}}{(E-\varepsilon_\lambda)\ (E-\varepsilon_{\lambda'})}$$

$$= \sum_\lambda \frac{C_\lambda}{E-\varepsilon_\lambda} \qquad (15)$$

which are essentially the formulae of Bethe [Be37]. The second term of (15) introduces some interferences between resonances which cancel each others in the case of capture (many channels - statistical hypothesis). As in the preceding case, the

U matrix is not unitary, due to the truncation process used. The total cross section is calculated from the sum of partial cross sections :

$$\sigma_t = 4\pi \lambda^2 \sum_{j s \ell} g_j \left\{ \sin^2 \phi_\ell + \cos 2\phi_\ell \sum_\lambda \left(\frac{\Gamma_n}{\Gamma}\right)_\lambda \frac{1}{1+X_\lambda^2} + \sin 2\phi_\ell \sum_\lambda \left(\frac{\Gamma_n}{\Gamma}\right)_\lambda \frac{X_\lambda}{1+X_\lambda^2} \right.$$

$$\left. + \sum_\lambda \sum_{\lambda' \neq \lambda} \frac{X_\lambda X_{\lambda'} + 1}{(1+X_\lambda^2)(1+X_{\lambda'}^2)} \left[\left(\frac{\Gamma_n}{\Gamma}\right)_\lambda \left(\frac{\Gamma_n}{\Gamma}\right)_{\lambda'} + \sum_{\alpha \neq n} \left(\frac{[\Gamma_n]^{1/2} [\Gamma_\alpha]^{1/2}}{\Gamma} \right) \left(\frac{[\Gamma_n]^{1/2} [\Gamma_\alpha]^{1/2}}{\Gamma} \right) \right] \right\} \quad (16)$$

The first part of the 4th term represents a scattering interference between resonances. These formulae are sometimes used for non fissile nuclei, taking in account only the resonance scattering interferences - as in the program MLBW [Gr 65].

1.2.4. Calculation by matrix diagonalisation. Several attempts have been done to diagonalize the matrix to be inverted in order to have an easy inversion ; as a fact, this is the method used by Adler and Adler to derive their formalism (see below). But the R matrix parameters are then lost. Some researches are being done at Saclay on a similar method which would allow to determine directly the R matrix parameters from a least square calculation (see annexe).

I.3. The "Kapur-Peierls" formalism was the first rigorous one [Ka 38]. It allows to express U as a sum over the resonances :

$$U \sim \sum_\lambda \frac{|\theta_\lambda\rangle \langle\theta_\lambda|}{H_\lambda - E}$$

where θ_λ and H_λ can be obtained from γ_λ and E_λ by a matrix transformation and are implicitly energy dependent ; for this reason the R matrix formalism has been preferred for a long time.

But since 1963 Adler and Adler [Ad 63] have been proposing a modified form of this formalism which is suitable for fissile nuclei resonance analysis. With this "Adler Adler formalism" the analysis of cross section of fissile nuclei is easier than with others ; it is not necessary to define the interfering levels. There is no simple relation between the parameters, and it is difficult to extract the R ma-

trix parameters. A method is being developed which allows one to obtain the R matrix parameters at least for a few levels [Ad 70] ; but it is not clear how well the interfering levels can be assessed.

I.4. The "S matrix formalism" developed by Humblet and Rosenfeld [Hu 61] following Siegert [Si 39] has the great advantage to give a "natural" definition of resonances with energy independent parameters, and simple formulae. But it does not give an automatic unitarity, which has to be introduced by conditions between parameters. Furthermore, the partial widths are such that : $\sum_{\alpha} \Gamma_{\alpha\lambda} \leq \Gamma_{\lambda}$.

I.5. Last, we must mention the phase shift analysis method. When there is only one channel : $U_{s\ell j} = e^{2i\delta_{s\ell j}}$.

It is not at present utilized to represent evaluated data, but is being used to analyze experimental data (scattering mainly) for light and medium nuclei, and cannot be ignored by evaluators.

II. APPLICATION OF THESE FORMALISMS.

According to the nucleus in question, a limited number of formalisms are used.

1). The "Breit and Wigner single level formula" is used as a first guess in nearly all the cases. It represents a good approximation for nuclei with $\overline{\Gamma}/\overline{D} < 0.1$, which is the most common case. It does not work properly for fissile nuclei and in the ten keV range (for light and medium nuclei like Fe, Ni, Cr ...).

2). The approximate formulae (13 and 16) are used to improve the analysis for nuclei with $\overline{\Gamma}/\overline{D} \lesssim 0.1$. In particular, by taking into account the scattering interferences, they allow some spin identification. For instance, Hibbon [Hi 59] has analyzed, with the MLBW formula, the total cross section of Al and Na up to $\sim$ 400 keV and has obtained some "appreciable mutual interference effects". It is probably a limiting case : for Al, he obtained for many couples of levels $\sqrt{\Gamma_1 \Gamma_2}/(E_2-E_1) = 0.6$ to 0.7. A better approximation is probably necessary in such cases.

3). The exact R matrix formulae for one channel is commonly used for nuclei with $\Gamma_\gamma << \Gamma_n$, such as structural materials. However the capture cross section of these materials, though it is small compared with the scattering, is important for reactors.

4). Since a few years the multilevel formalisms (Reich Moore or Adler Adler) are intensively used for fissile nuclei data analysis. But in most cases the application of the Reich Moore formalism, which requires an explicit definition of the interfering levels, is done with only one fission width for each level. In most of the analysis done in Los Alamos, the resonances are classified in 4 groups. The fission widths of each group should follow a χ^2 law with ν=1. In fact, it is experimentally found that they are distributed according to χ^2 laws with ν=3 to 5 [Ri 70]. This means that the multilevel description is not physically meaningful.

5). The Humblet Rosenfeld formalism was used a few years ago for the analysis of light nuclei data. But it has never been used for evaluation, and recent studies, on ^{6}Li for instance, are made in the frame of the R matrix formalism.

III. METHODS USED TO EVALUATE THE RESONANCE PARAMETERS.

The natural way is to use the published resonance parameters. This supposes at least that the various authors : i) use the same formalism, ii) identify at least the same prominent levels (there may be some differences for small ones).

This is obviously not the case for the fissile nuclei. The comparison - and then the direct evaluation - of the parameters is in practice possible when :

- either the Breit and Wigner single level, or the MLBW formalism are used (their results can be compared) ;
- or there is only one channel and the data are analyzed with the same formalism.

In the other cases, which are mainly the fissile nuclei, the evaluator have the choice between two solutions : i) to adopt one of the existing sets, without taking the others into account ; ii) to reanalyse the data from various laboratories.

Even if several authors are using the same formalism to analyse the same data for fissile nuclei, it is possible to obtain different sets of parameters. This is due to the "non uniqueness" of the multilevel fits. It is generally accepted that this "non uniqueness" is due to uncertainties in the experimental data and to the fact that the distance levels are not taken into account ; but according to recent calculations by Auchampaugh [Au 71] its origin could be more fundamental : it could exist even for few levels without experimental errors.

In all the cases the evaluator have to check the average cross sections calculated from the parameters with the experimental average values.

IV. THEORIES USED IN THE INTERPRETATION OF RESOLVED RESONANCE PARAMETERS

The analysis of the resonance parameter distributions allows us to check the theoretical laws and to determine the average parameters. These laws and the consequent average values are useful in the statistical model calculations. The laws are well known.

IV.1. Spacing.

Many studies have been made in past which all conclude that the Wigner law :

$$\rho_{(x)}\, dx = \frac{\pi}{2} \times e^{-\pi/4\, x^2}\, dx$$

with $x = D/\overline{D}$ is a very good approximation of the spacing distribution law. The problem rather concerns the existence of correlations between spacings which are predicted by theories and have been experimentally observed. For the commodity of discussion, we can share these correlations in two categories :

a) The short range correlation. The correlation between two adjacent spacings (D_i and D_{i+1}) is about - 0.2. The effect of this correlation will be to narrow the distribution of the spacing between levels λ and $\lambda+2$. Is it important to take this correlation into account in simulating cross sections ? It has not been done up to now. As there exists always a superposition of many independent populations of levels with different spins and parities, one may expect that the influence of this correlation will be of the second order.

b) The long range correlation. There exists a negative long range correlation ; its effect is to regularize the number of levels in a given energy range. According to Dyson and Mehta [Dy 63], the variance of the number of levels in a given energy range is :

$$\sigma_N^2 = \frac{2}{\pi^2}\left[\text{Log}\ (2\pi N) + 1 + \gamma - \frac{\pi^2}{8}\right] = 0.206\left[\text{Log}\ (2\pi N) + 0.343\right] ;$$

The following table gives some values.

Average number N of levels in energy range ΔE		10	30	100	300	1000
relative standard deviation on N according to	the Wigner law without any correlation	16,5%	9,5%	5,2%	3,0%	1,65%
	Dyson and Mehta [Dy63]	9,5%	3,5%	1,17%	0,42%	0,136%
	a χ^2 law - distribution with ν=1.	44,7%	25,8%	14,1%	8,2%	4,5%

From this we may conclude that the fluctuations of average cross section will be due mainly to partial width fluctuations.

IV.2. Widths.

The reduced width γ^2 is distributed according to a χ^2 law with one degree of freedom. This is usually the case of the neutron reduced width $\Gamma_n^{\ell *}$.

The other partial widths are generallv the sum of several (or many) reduced widths having different average values. They are distributed according to a χ^2 law only in the case where all the reduced widths have the *same* average value. This never happens in practice. Then the usual way to describe a partial width distribution by a χ^2 law with ν_{exp} degrees of freedom is just a convenient one and does not correspond to the number of channels which is always greater than ν_{exp}.

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* It has to be noticed that $\Gamma_n^{\ell,J}$ for $\ell > 1$ may result from the addition of two or more reduced widths corresponding to different channel spins.

We can consider two problems :

a) *Number of degrees of freedom.* It is commonly accepted that ν is equal to 1 for a partial width. Indeed many analyses give, for the neutron width distribution, a value of ν which is slightly greater than 1, but there is not enough evidence to conclude on this problem. On the other hand there are great discrepancies on the value of ν_{exp} for the fissile nuclei according to different experiments.

It is known that :

$$\overline{\sigma_{n,\alpha}} = \frac{\overline{\Gamma_n}\ \overline{\Gamma_\alpha}}{\overline{\Gamma}}\ S_{n,\alpha}$$

with :

$$S_{n,\alpha} = \frac{< \dfrac{\Gamma_n\ \Gamma_\alpha}{\Gamma} >}{\dfrac{\overline{\Gamma_n}\ \overline{\Gamma_\alpha}}{\overline{\Gamma}}}$$

Let us suppose that we know exactly the average values of the parameters ; the error on $\overline{\sigma_{n,\alpha}}$ is due to the error on $S_{n,\alpha}$ then to the errors on the distribution laws. We can ask two questions :

1) What is the variation of $S_{n,\alpha}$ if ν, for the neutron width distribution law, is not exactly equal to 1 ? The table 1 gives an answer to this question.

Table 1

Influence of the exact value of ν_n (number of degrees of freedom of the reduced neutron width distribution) on the values of $S_{n,n}$ (upper value) and $S_{n,\alpha}$ (lower value).

$\overline{\Gamma}_n$ (eV)	0.01		0.06		0.21	
$\overline{\Gamma}_\alpha$ (eV)	0.04		0.04		0.04	
ν_n	1	1.2	1	1.2	1	1.2
$\nu_\alpha = 1$	2.78 0.555	2.71 0.573	1.330 0.505	1.314 0.529	1.081 0.577	1.075 0.606
$\nu_\alpha = 4$	2.14 0.714	2.05 0.738	1.252 0.622	1.231 0.654	1.063 0.671	1.056 0.706
$\nu_\alpha = \infty$	1.85 0.786	1.75 0.812	1.213 0.681	1.189 0.716	1.054 0.716	1.047 0.754

It appears that a 20% increase on ν_n induces a 1 to 5% decrease on $S_{n,n}$ and a 4 to 6% increase on $S_{n,\gamma}$.

2) What is the variation of $S_{n,\alpha}$ with the number of degrees of freedom for a fission width distribution law ? An answer is given in the next table.

Table 2

Influence of the equivalent number of degrees of freedom for the fission width distribution on the value of $S_{n,n}$, $S_{n,f}$ and $S_{n,\gamma}$. We suppose that Γ_γ = 0.04 eV = constant, ν neutron = 1.

$\overline{\Gamma}_f$ (eV)	0.02		0.1		0.5	
$\overline{\Gamma}_n$ (eV)	0.01	0.1	0.01	0.1	0.01	0.1
$S_{n,n}$ for ν_f = 2	2.123	1.199	3.033	1.496	5.333	2.576
$S_{n,n}$ for ν_f = 3	2.102	1.197	2.863	1.473	4.462	2.406
$S_{n,n}$ for ν_f = 4	2.090	1.196	2.766	1.461	4.017	2.313
$S_{n,f}$ for ν_f = 2	0.708	0.622	0.725	0.589	0.835	0.669
$S_{n,f}$ for ν_f = 3	0.740	0.639	0.774	0.621	0.882	0.712
$S_{n,f}$ for ν_f = 4	0.759	0.648	0.802	0.639	0.905	0.736
$S_{n,\gamma}$ for ν_f = 2	0.866	0.692	1.180	0.788	1.979	1.201
$S_{n,\gamma}$ for ν_f = 3	0.854	0.688	1.099	0.764	1.616	1.080
$S_{n,\gamma}$ for ν_f = 4	0.848	0.687	1.054	0.751	1.435	1.015

From this table we can see that if the exact value of ν_{eq} has only a small importance when Γ_f is small, the effect cannot be disregarded when Γ_f is great.

b) *Influence of correlations*. Let us suppose that there is an "important" correlation between Γ_γ and Γ_n, for instance that :

$$\Gamma_\gamma = \text{constant} + \varepsilon\, \Gamma_n .$$

In this case the correlation coefficient r is always equal to 1 whatever may be $\varepsilon(>0)$. The knowledge of the correlation coefficient is not sufficient

to determine the importance of a correlation. It is necessary to introduce a quantity such as :

$$A_{cor} = \frac{[\text{var } \Gamma_1 \text{ var } \Gamma_2]^{1/2}}{\overline{\Gamma}_1 \overline{\Gamma}_2}$$

If the distribution of the width is described by χ^2 law , the amplitude of correlation is :

$$A_{cor} = \frac{2}{\sqrt{\nu_1 \nu_2}} .$$

Of course, this is an extreme case. Let us consider the following more realistic case. We suppose that :

$$\Gamma_\gamma = V + \varepsilon \Gamma_n$$

where V is a random quantity, independent of Γ_n, and distributed according a χ^2 law with ν_V degree of freedom ; Γ_n follows the same law with 1 degree of freedom. In the table 3 we consider four values of the couple $(\overline{\Gamma}_n, \overline{\Gamma}_\gamma)$ chosen in such a way that :

$$\frac{\overline{\Gamma}_n \overline{\Gamma}_\gamma}{\overline{\Gamma}_n + \overline{\Gamma}_\gamma} = \text{constant} = 0.0075 \text{ eV}.$$

We give the value of $S_{n,\gamma}$ when there is no correlation between Γ_n and Γ_γ ($\varepsilon = 0$), and when there is a correlation ($S^n_{n,\gamma}$). The values of $\overline{\Gamma}_n$, $\overline{\Gamma}_\gamma$, V and ε are such that :

$$r(\Gamma_n, \Gamma_\gamma) = \text{constant} = 0.326.$$

We characterize the distribution of the radiation width by :

$$\nu_{eq} = \frac{2 \overline{\Gamma}^2_\gamma}{\text{Var}(\Gamma_\gamma)} .$$

Table 3

Value of $S_{n,\gamma}$ with and without a realistic correlation ($r(\Gamma_n, \Gamma_\gamma) = 0.326$). All the widths are expressed in eV.

	ν_V	5.02	23.3	100	413.9
	$A(\Gamma_n,\Gamma_\gamma)$	0.818	0.409	0.2045	0.1023
	ν_{eq}	5.98	23.9	95.6	383
Values of $\overline{\Gamma}_n$ and $\overline{\Gamma}_\gamma$ (eV)	$\overline{\Gamma}_n = 0.04$ $\overline{\Gamma}_\gamma = 0.00923$	V = 0.008 $\varepsilon = 0.0307$ $S^c_{n,\gamma} = 0.689$	V = 0.00862 $\varepsilon = 0.0153$ $S^c_{n,\gamma} = 0.707$	V = 0.00892 $\varepsilon = 0.00769$ $S^c_{n,\gamma} = 0.709$	V = 0.00908 $\varepsilon = 0.00384$ $S^c_{n,\gamma} = 0.708$
		$S^u_{n,\gamma} = 0.673$	$S^u_{n,\gamma} = 0.697$	$S^u_{n,\gamma} = 0.704$	$S^u_{n,\gamma} = 0.706$
	$\overline{\Gamma}_n = 0.02$ $\overline{\Gamma}_\gamma = 0.012$	V = 0.0104 $\varepsilon = 0.08$ $S^c_{n,\gamma} = 0.658$	V = 0.0112 $\varepsilon = 0.04$ $S^c_{n,\gamma} = 0.680$	V = 0.0116 $\varepsilon = 0.02$ $S^c_{n,\gamma} = 0.682$	V = 0.0118 $\varepsilon = 0.01$ $S^c_{n,\gamma} = 0.682$
		$S^u_{n,\gamma} = 0.641$	$S^u_{n,\gamma} = 0.670$	$S^u_{n,\gamma} = 0.680$	$S^u_{n,\gamma} = 0.680$
	$\overline{\Gamma}_n = 0.01$ $\overline{\Gamma}_\gamma = 0.03$	V = 0.026 $\varepsilon = 0.4$ $S^c_{n,\gamma} = 0.752$	V = 0.028 $\varepsilon = 0.2$ $S^c_{n,\gamma} = 0.769$	V = 0.029 $\varepsilon = 0.1$ $S^c_{n,\gamma} = 0.768$	V = 0.0295 $\varepsilon = 0.05$ $S^c_{n,\gamma} = 0.765$
		$S^u_{n,\gamma} = 0.711$	$S^u_{n,\gamma} = 0.747$	$S^u_{n,\gamma} = 0.757$	$S^u_{n,\gamma} = 0.759$
	$\overline{\Gamma}_n = 0.008$ $\overline{\Gamma}_\gamma = 0.12$	V = 0.104 $\varepsilon = 2$ $S^c_{n,\gamma} = 1.138$	V = 0.112 $\varepsilon = 1$ $S^c_{n,\gamma} = 1.057$	V = 0.116 $\varepsilon = 0.5$ $S^c_{n,\gamma} = 0.996$	V = 0.118 $\varepsilon = 0.25$ $S^c_{n,\gamma} = 0.955$
		$S^u_{n,\gamma} = 0.865$	$S^u_{n,\gamma} = 0.894$	$S^u_{n,\gamma} = 0.901$	$S^u_{n,\gamma} = 0.885$

We can see that the effect of a correlation between Γ_γ and Γ_n upon $S_{n,\gamma}$ is important when either the variance of the Γ_γ width distribution or the ratio $\overline{\Gamma}_\gamma/\overline{\Gamma}_n$ are great. Then such a correlation may have important consequences for p wave or d wave neutrons.

V. *DEPENDENCE ON ℓ, J and E OF THE AVERAGE PARAMETERS*

This is a very wide matter which cannot be considered here. We shall just note a few points :

V.1. Strength functions.

a) It has to be remembered that, for $\ell \geq 1$, they are meaningless if the nuclear radius used is not defined.

b) Some spin dependences have been claimed by various authors ; but most of the time the differences observed can be explained only by the sampling errors, without taking into account the experimental ones.

c) Variation with A. The optical model predicts the gross variation. But some fine variations have been observed for Sn, Xe, Te which can be explained by shell model [Sh 63] or by introducing an isospin potential term [Ne 71].

V.2. Spacing.

According to the frame of present theories, the knowledge of the variation of $\overline{D}$ with J is limited by the one of σ^2, the spin cut off factor ; and, with energy, by the knowledge of a. The average spacing is not correctly predicted, at present time, by theories.

V.3. Radiation width.

It is usually accepted that it is independant of spins and parities. But there is some evidence of a spin (or parity) effect mainly in the case of even-even compound nuclei, which have a simpler level scheme than the other nuclei.

V.4. Fission width.

Until the year 1968, many works have been done to interpret the fission width distribution by the channel theory of Bohr and Wheeler. Some reviews of the interpretation were presented at Conferences in 1965 [Gr 65, Ly 65] and 1966 [Ly 66]. Since that time the discovery of the subthreshold fission has changed considerably the nature of the problems to be solved and has increased the interest of nuclear physicists in fission.

VI. UNRESOLVED RESONANCES - ANALYSIS AND INTERPRETATION

It is common sense that the average experimental cross sections have to be equal to the calculated ones. If it is not so, this signifies that the averaged parameters utilized are not correct ; up to now it has not appeared that there were some important reserves on the theoretical background (except of course for non statistical effects).

But what does "average" mean ? It is obvious that if the averaging is done on a too small energy range there will be some fluctuations which are meaningless for the average cross section. These fluctuations are related to the statistical laws, and can be compared with their predictions.

The first attempt in this sense is probably the one by Egelstaff in 1957 [Eg 57]. Several studies follow this method, in particular to set up evidence for correlations. But it has been shown [Pe 69] that we have to be very cautious in the interpretation of the correlogramms.

A new approach to the study of the cross section fluctuations has been recently given by James ; it is based on "Wald and Wolfowitz" distribution free statistics, and was applied to resonance parameters as well as to cross section data points [Ja 70,71].

It is possible to conceive another way to approach this problem ; the probability distribution of cross section, $P(\sigma)$, (see VII), for various temperatures can be obtained directly from experimental data by artificially broadening the resolution. This distribution can be characterized by its first momentum, whose theoretical values can be calculated from distribution laws.

Intermediate structures.

Since the beginning of the years 60 it has become usual, for nuclear physicists, to claim that their results show some "possible" doorway state or intermediate structure.

On the other hand, Mahaux et al. [Ma 69] concluded that "the experimental data themselves contain *no* information which could indicate that a doorway state mechanism is actually operative. There exists no way of analyzing the fine structure nor the energy averaged data which could prove or disprove the presence of a doorway state. This corresponds to the fact that the definition of a doorway state is model dependent".

They concluded that, for instance, there is no proof of the existence of such structures in the reactions $^{56}Fe(n,n)$ and $^{208}Pb(p,n)$. They recognized that intermediate structures exist with certitude in a few cases :

- the photonuclear giant resonance
- the isobaric analogue resonances
- the subthreshold fission resonances grouping (^{237}Np, ^{240}Pu).

Many cases of intermediate structures have been obtained in fission (^{234}U, ^{239}Pu). But it is necessary to be very careful before accepting them.

VII. IMPORTANCE OF INTERFERENCES AND INTERMEDIATE STRUCTURES FOR REACTORS

Let us suppose that the average cross section is well evaluate in all the cases. Then the fact of taking into account the interferences or structures will only change the shape of the cross sections, and may introduce some variations in :

- self shielding
- Doppler effect.

There are only a few studies on these problems.

Interferences. One may expect that there will be only a small change of the self shielding.

The influence on the Doppler effect has been studied by Menapace et al. [Me 67] in a simple case : only two interfering levels for a fissile nuclei, and an isolated level for a fertile nuclei. They had many parameters : spacing d between the 2 fissile levels, spacing D between the fertile nuclei level and

one of the fissile nuclei levels, etc ... They calculated the variation of the effective integral I between T = 300°K and T = 600°K for 1 keV neutrons, gave the relative value of this change versus D for 1 or 2 values of d, and averaged over D in one case (^{233}U - ^{232}Th). But they normalized the variation of I to an unknown quantity Io, and they did not integrate over all the probability distributions of all the parameters and one can hardly conclude on the effects of the interferences.

Fluctuations and intermediate structures. Let us suppose that, at a given energy E, we know the experimental average cross section $\overline{\sigma}_{n,\alpha}$. It is generally different from the one which is calculated from the average parameters, $\langle\sigma_{n,\alpha}\rangle$ and from the others which may be calculated from various sets of random parameters, drawn up by using these average parameter values. Is it necessary to adjust these average values to adjust the calculated cross sections to the experimental value ?

A possible answer may be :

- if we know that the experimentally observed fluctuation is not due to an intermediate structure, but just to statistical fluctuations, then we have to use the average parameters.

- on the contrary, if we know that there is an intermediate structure, we have to modify in consequence the average parameters.

Intermediate structures. We shall refer to the study by L'Heriteau and Neviere [Lh 71] who considered the effect of possible sub-threshold fission in ^{240}Pu and ^{239}Pu.

For ^{240}Pu the variation of the self shielding coefficient for fission is small (2% at 300°K for a dilution of 50 barns) while the Doppler effect coefficient for fission increases by 40%. For ^{239}Pu, the self shielding coefficient changes by less than 1.5% but the introduction of the intermediate structures increases slightly the Doppler effect for capture (1 or 2%) and decreases significantly the one for fission (10 to 30%).

Conclusion. We cannot conclude on the effect of interferences ; the effects of intermediate structures may be important on Doppler effect. In both cases more studies are necessary.

VIII. REPRESENTATION OF RESONANCE DATA

The reactor physicist is interested by the distribution of probability $P(\sigma_{n,\alpha})$ of $\sigma_{n,\alpha}$ at given energies and temperatures. It can be formaly related to $\sigma_{(E)}$ by :

$$\int \sigma\, P(\sigma_{n,\alpha})\, d\sigma_{n,\alpha} = \sum_{\ell,J} \int_{\text{parameters}} \sigma_{n,\alpha}\,(\ell,\ J,\ \text{sum over levels})\ P_{(\text{par.})}\ d_{(\text{par.})}$$

where $\sigma_{n,\alpha}\ (\ell, J, \sum_{\lambda})$ is the cross section taking into account many levels. Then we can, in principle, represent resonance data (both in resolved and unresolved range) by three methods :

a) by giving $\sigma_T(E) = f(E)$ (T is for temperature)

b) by giving the resonance parameters

c) by giving the $P_{(T,E)}\ (\sigma)$ law.

First method. $\sigma_T(E) = f(E)$

It is of course temperature dependent, and requires a great number of points.

a) It can be used in the resolved resonance range, because the data are meaningful and the number of resolved levels is limited (< 300). At Saclay we give this curve for a T = 0°K temperature with 13 points by resonance.

b) In the unresolved field it is necessary to draw out random parameters (from the known statistical laws) and to compute the cross section $\sigma_T(E)$ which is only statistically meaningful : the calculated cross section is generally not equal to the actual value. According to the research accuracy, it can require a great number of levels and many more data points for each temperature and each energy considered.

This representation, which is not convenient, is not very much used ; we must notice, nevertheless, that it is utilized in UK in the GENEX system.

Second method. Resonance parameters. They are essentially temperature independent.

a) It is the most natural representation in the resolved energy range.

b) In the unresolved field, the parameters of individual resonances are necessary if one wants to compute the cross sections and constitute a sufficiently compact representation of the information - which can be extracted only by computing the cross sections (except if one is only interested in the average - but then it is not necessary to draw up the random parameters).

Third method. It is a temperature dependent, but very compact way to represent the data.

a) This compactness is probably not true if one requires a great accuracy in the resolved resonance range, especially at low energies.

b) The advantage of this method exists mainly in the unresolved range.

Conclusion. It seems that the resonance representation can be better made :

a) in the resolved resonance range, by utilizing the individual resonance parameters.

b) in the unresolved range, by utilizing :

- the average parameters and their statistical laws
- for several temperatures T, the probability of σ.

The problem is the calculation of $P(\sigma)$.

Remarks on $P(\sigma)$. The representation of the cross section fluctuations by $P(\sigma)$ is, in fact, the basis of the "sub groups" method of Nikolaev et al. [Ni 70, Ni 71].

The calculation of $P(\sigma)$ is probably impossible ; but this distribution can be characterized by its momentum, which may be calculated from the probability distributions of the resonance parameters - at least in the case of the Breit and Wigner single level formula.

ANNEXE

On peut montrer que l'élément $U_{n\alpha}$ de la matrice de collision, en tenant compte des interférences entre les niveaux, est de la forme :

$$U_{n\alpha} = \sum_{\lambda} \frac{\beta_{n\lambda}\ \beta_{\alpha\lambda}}{\mathcal{E}_{\lambda} - E}$$

$$\beta_{\alpha\lambda} = \sum_{\mu} \gamma_{\alpha\mu}\ V_{\mu\lambda}$$

$V_{\mu\lambda}$ et $\mathcal{E}_{\lambda}$ sont respectivement les composantes du vecteur propre $\mathbb{V}_{\lambda}$ et la valeur propre correspondante de la matrice de niveaux A^{-1} à l'énergie E=0. Ces quantités sont indépendantes de l'énergie, tout au moins si Γ_t et les éléments non diagonaux de A sont indépendants de l'énergie. Ainsi la section efficace $\sigma_{n\alpha}$ peut s'écrire :

$$\sigma_{n\alpha} = \frac{C}{\sqrt{E}} \sum \frac{C_{\lambda}}{\mathcal{E}_{\lambda} - E} + \frac{C_{\lambda}^{*}}{\mathcal{E}_{\lambda}^{*} - E}$$

où C_{λ} est indépendant de l'énergie.

Pour l'analyse par moindres carrés des sections efficaces mesurées, on est amené à calculer les dérivées des sections efficaces.

Si on utilise la propriété suivante :

$$\frac{\partial A}{\partial x} = - A \frac{\partial A^{-1}}{\partial x} A$$

où A est une matrice dépendante du paramètre x, on montre que cette dérivée peut s'écrire :

$$\frac{\partial \sigma}{\partial x} = \frac{C}{\sqrt{E}} \sum_{\lambda} \left(\frac{CD_{\lambda}}{\mathcal{E}_{\lambda} - E} + \frac{CDD_{\lambda}}{(\mathcal{E}_{\lambda} - E)^2} \right) + \text{complexe conjugué}$$

CD_{λ} et CDD_{λ} sont indépendants de l'énergie ; x est un des paramètres de la matrice R : E_{λ}, Γ_t, γ_n°, γ_f ...

Ainsi, les formes analytiques de σ et $\frac{\partial \sigma}{\partial x}$ étant simples, il est facile de convoler ces fonctions par les fonctions représentant l'élargissement Doppler et la résolution.

Les paramètres utilisés sont ceux de la matrice R. Ce sont eux qui sont ajustés par moindres carrés. Les paramètres β_λ, $\Im_\lambda$ ne sont considérés que comme des intermédiaires de calcul. Le calcul des coefficients CD_λ et CDD_λ de $\frac{\partial\sigma}{\partial x}$ est assez compliqué mais certaines approximations peuvent être faites, compte tenu des approximations inhérentes à la méthode de moindres carrés.

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ENERGY REGION OF RESOLVED AND UNRESOLVED RESONANCES

THE ACTIVITY OF THE CNEN NUCLEAR DATA GROUP IN BOLOGNA, ITALY

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Abstract

The CNEN Italian activities concerning the resonance region of the neutron cross sections are shortly summarized.

Some critical questions and needs are also pointed out, involving the experimental and theoretical analysis of the resonances and the problems of the multilevel representation.

1. PRESENT STATUS AND FORMALISMS USED

The activity of the CNEN Nuclear Data Group for the evaluation of neutron cross sections in the resonance region includes some studies on the multilevel formalism and its consequences in the calculations of the Doppler effect in fast reactors.

The shielding effect among resonances of fissile and fertile materials was early studied in connection with the problem of the temperature variation of the resonance integral. A two-level formula was adopted for the case of two interfering resonances of the fissile material overlapping with one resonance of the fertile material.

The temperature variation of the resonance integral resulted to be not very largely influenced by the formalism [1]. However, the calculation with a two-level formalism showed that the change in the resonance integral due to the attribution of a constructive or destructive interference between levels greatly overcomes any change due to the temperature effect [2].

The fact seemed relevant enough to encourage deeper studies on the role played by all the possible combinations of interference in the mathematical expression of a multilevel formalism.

The Reich-Moore and Adler-Adler formalisms did not seem easy to handle for a study on the effect of a large number of interference combinations among resonances.

The origin of a proper type of interference in a multilevel cross section representation lies mathematically in the fact that the reduced width parameters are signed quantities. Our effort was therefore devoted to the preparation of a multilevel two-channel formula, suitable for computer calculations of the interferential effects among resonances as generated by the sign attribution. The requirement was attained to reproduce some formulas of the above mentioned formalisms, in known cases.

The approach has successively been extended to the multilevel many-channel case [3]. However, a good settlement of such work would require further criticism and discussions.

2. EXPERIENCES, LIMITATIONS AND ACHIEVEMENTS IN THE APPLICATION OF THEORY TO RESOLVED RESONANCE PARAMETERS

In order to estimate the unknown resonance parameters of some isotopes, the up-to-date values of Γ_γ and D observed for nuclides with mass number between 45 and 210 were collected.

The D_{obs} values will be used to compile a systematics of the level density parameter "a", of a Fermi gas formula. Such a work is now in progress taking into account the rotational energies of the nuclei.

For what concerns the analysis of the experimental data, it is our opinion that a greater attention must be paid to the evaluation of the response function of the experimental apparatus and the criticism on the unfolding method.

For a better resolution of the widely overlapped resonances the shape analysis would be preferable to the area analysis, in order to avoid too large errors in the evaluation, especially of the neutron widths.

Any effort for the improvements of the theoretical approximation (Breit--Wigner, multilevel, etc.) would be unfruitful if the above conditions were not satisfied.

3. ENERGY AND SPIN-DEPENDENCE AND SYSTEMATICS OF AVERAGE RESONANCE PARAMETERS

The spin-dependence of the level mean spacing in hafnium isotopes has been recently studied by resonance neutron capture experiments [4].

In order to check the spin-dependence of the s-wave strength function, its values were determined, as deduced from the analysis of the low energy data in the 177 and 179 Hafnium isotopes [5].

No definite conclusions were reached about the question (which was also touched upon last year at the Helsinki Conference), especially for the mentioned uncertainties in the Γ_n^o measurements.

4. IMPORTANCE OF RESONANCE INTERFERENCE AND INTERMEDIATE STRUCTURE IN FISSION ON THE DOPPLER EFFECT

Following the criteria mentioned in 1, an application was made of the multilevel two-channel formula in order to determine the effect in the cross section value due to the signs of the reduced width amplitudes [6].

The fortran code PIUME [7] is now available for the calculation of the two-channel case. It utilizes the input real parameters of the R-matrix formalism. For a direct comparison of the results, it would be desirable to have Reich-Moore and Adler-Adler tested codes.

It is also our need to have the original conversion programs of parameters for the different formalism, as for example the Gamplex code (Helsinki Conf. 1970).

In the evaluation of the importance of resonance interference, single and two-level formulas were used in some of the codes set up in Centro di Calcolo, which calculate group cross sections in resolved and unresolved region. The detailed description of the codes will be found in the reports [8], [9], [10], [11].

5. REPRESENTATION OF RESOLVED AND UNRESOLVED RESONANCE DATA

The resonance cross section representation in the Nuclear Data Files is generally provided either in tabulated form or through the parameters of a specified formalism.

The tabulated form sometimes requires a very high number of points, with some difficulties for the Doppler broadening by numerical methods (e.g. TEMPO code) in the resolved region. Moreover, the temperature dependence in the unresolved region cannot be calculated. The repetition of data for different temperatures would probably enlarge too much the Nuclear Data File.

The parameter representation, in many cases, implies the addition of a background value, step-variable. For a correct calculation of the cross section temperature dependence the handling criteria of such background data in the Doppler broadening must be given or the determination method explained.

When a choice of the representation is possible, the preference for a parameter representation depends, in our opinion, upon the availability of standardized codes for the Doppler broadening. An agreement upon the procedure for the generation by the mean parameters of the temperature dependent cross sections in the unresolved region would be desirable.

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RESEARCH OF THE BEST RUNNING CONDITIONS OF NUCLEAR CODES FOR COUPLED CHANNEL CALCULATION OF NEUTRON INTERACTION WITH HEAVY DEFORMED NUCLEI

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Abstract : *The effects of various physical approximations in the coupled channel optical model and the errors due to the uncertainty in the deformation parameters were examined.*

As for the shape of potential, we must consider the deformation of imaginary potential but can neglect the deformation of spin-orbit coupling potential. The deformed potential should be expanded with Legendre polynomials at least up to $\lambda = 4$.

When the energy of the incident neutron is less than 1 MeV, the coupling of 3 levels seems most reasonable except for the inelastic scattering. The errors in cross sections are less than 3 % with this condition. For calculating the inelastic scattering to the n-th state, the coupling to the (n+1)-th state is required. If the neutron energy is higher than 1 MeV, the adiabatic approximation is highly recommended, because more precise results can be obtained with much less computing time.

In the coupled channel model, we must consider the contributions of high angular momentum which are negligible in the spherical optical model.

The uncertainties of the deformation parameters cause considerable errors. The uncertainty of β_2-value is ± 10 % and that of β_4-value is a complete open question. Hence the errors due to these uncertainties are inevitable, even if the errors due to the physical approximations can be removed. The errors are estimated to be 3 % for the reaction and the elastic scattering cross sections, 5 % for the strength functions and 20 % for the inelastic scattering cross sections, respectively.

I - INTRODUCTION

The optical model is often used to analyze cross sections, angular distributions, polarizations and strength functions and also to obtain the transmission coefficients needed for the statistical model calculations. The best set of the optical model parameters is searched for in order to obtain the best fit of the experimental data. Before doing so, however, we must check the reliability of the calculated results and know the limit of the errors. The purpose of this report is to examine these problems which must be solved before searching for the best optical model parameters.

Two types of errors can be considered. The first one is the error due to the numerical calculation in the program, such as the truncation error, the round-off error and the error due to the finite matching radius. The conditions of numerical integration must be chosen very carefully. The basic physical constants, such as the neutron mass, the conversion constant between energy and wave number must be also checked. These problems were examined for the spherical optical model code in the preceding report [1] and the best conditions were recommended.

The second type of error is caused by various physical assumptions adopted in the calculation. This type of error is much more complicated in the coupled channel optical code, because we have so many optional assumptions. Hence we mainly discuss the effects of these various physical assumptions in this report.

The effects of the values of deformation parameters are also discussed, because these values are generally assumed before searching for the best optical model parameters. The uncertainty of the deformation parameters causes considerable errors on the results. This uncertainty seems to be ignored in most of the present analyses.

The general coupled channel optical model codes available at Saclay are ECIS 70 [2]* and JUPITOR [3]. The ADAPE [4] code, the program using the adiabatic approximation is also available. The results of these 3 codes were compared and were proved to agree with one another when the appropriate conditions are used (see section II.5 and appendix 1).

In the present examination, our efforts are devoted only to the interaction of ^{238}U with neutrons whose energies are 0.1, 0.6 and 2 MeV. However the present conclusion may be applied to the other heavy deformed even-even nuclide for reaction with neutrons whose energy is less than 15 MeV.

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* Raynal recently developed a new code ECIS 71 in which the automatic search is possible. However the principal part for solving the coupled equations is the same as ECIS 70.

II - EFFECT OF VARIOUS PHYSICAL APPROXIMATIONS

We must choose the following physical approximations :

1) choice of imaginary potential (deformed or spherical) ;

2) order of Legendre expansion of the deformed potential ;

3) choice of spin-orbit coupling potential (deformed or spherical) ;

4) number of coupled levels (for non-adiabatic case) ;

5) adiabatic approximation.

Among these five, the most interesting problems are the conditions 4) and 5), i.e., the influence of the numbers of the coupled levels for non-adiabatic case and the validity of adiabatic approximation. Therefore we will first discuss the conditions 1), 2) and 3) briefly and discuss the conditions 4) and 5) more precisely. The ECIS 70 code is mainly used for non-adiabatic case, because this code was found to be more rapid than the JUPITOR code. The comparison of these two codes will be discussed in appendix 1.

The parameters of the optical potential are tabulated in table 1. The mesh interval and the matching radius in the numerical calculation are taken 0.1 fm and 15 fm respectively. This condition was proved in ref.1 to give the precision of 10^{-3} in C matrix coefficients for a program with single precision on an IBM.360/91 computer.

We examine the effects of various approximations on the following values :

1) C matrix coefficients ;

2) s and p wave strength functions ;

3) integrated cross sections (reaction, elastic and inelastic scattering) ;

4) differential cross sections (elastic and inelastic scattering) ;

5) polarizations.

In order to compare the differential cross sections and polarizations, we define the relative deviation as :

$$\text{dev}\ (A) = \sqrt{\frac{\int\left(A(\theta) - A^{st}(\theta)\right)^2 d\theta}{\int\left(A^{st}(\theta)\right)^2 d\theta}}\ , \qquad (1)$$

where A is a set of differential cross sections or polarizations, and A^{st} the value of the standard set. This relative deviation is considered to be a good measure of the differences under various conditions.

In the following tables, values of C matrix coefficients are given only for the standard set and absolute differences from the standard values are given for the other sets in order to make comparison easier.

The so-called "standard set" varies from case to case according to the properties to be checked ; it will be defined in each case.

II.1 Effect of deformation of imaginary potential

The effects of deformation of the imaginary potential were examined with the coupling of 2 levels and with P4 expansion for incident neutrons with energy of 0.6 and 2 MeV.

The results with the spherical and the deformed imaginary potential are compared in table 2. The results with the deformed imaginary potential are taken as standard values.

The absolute errors in the C matrix coefficients are of the order of 10^{-2}. The relative errors on the strength functions and on the total reaction and elastic cross sections are less than 10 %.

Differential scattering cross sections and polarizations at 2 MeV are shown in fig.1. Considerable differences (factor of 2) are observed in the case of elastic scattering for $\theta > 120°$.

On the other hand, the difference of the time for computation is less than 20 %. Hence we conclude that the deformed imaginary potential should be employed.

II.2 Effect of order of Legendre expansion

The deformed potential is expanded with Legendre polynomials. The order of expansion should be $2 \times I$, if the spin of the highest coupled level in the ground state band is 1.

JUPITOR and ADAPE allow the expansion up to 4, though ECIS 70 allows a higher expansion. Here we compare the results with P2 ($\lambda = 2$ only), P4 ($\lambda = 2$ and 4) and P6 ($\lambda = 2$, 4 and 6) expansion with the coupling of 3 levels (0^+, 2^+ and 4^+) at 0.6 MeV and 2 MeV. They are tabulated in tables 3A and 3B in which P4 expansion is taken as the standard.

The absolute differences in the C matrix coefficients are of the order of 10^{-2} between P2 and P4 and less than 10^{-3} between P4 and P6. The differences in the cross sections and the strength functions are several percents between P2 and P4 and less than 1 % between P4 and P6. The differential scattering cross sections and polarization are shown in fig.2. A considerable difference is observed between P2 and P4 but very little difference between P4 and P6. The difference of the computing time is less than 15 %.

As a conclusion, P2 expansion should be abandoned, because it causes a considerable error. Theoretically the higher expansion should be recommended, but P4 expansion seems sufficient. In the following comparison, we will use P4 expansion in order to compare the results with those of JUPITOR and ADAPE in which the expansion is allowed up to $\lambda = 4$.

II.3 Effect of deformation of spin-orbit coupling potential

The spin-orbit coupling potential (V_{SL}) can be deformed in ECIS 70. The effects of this deformation are shown in table 4 and fig.3. The effects on the C matrix coefficients are of the order of 10^{-3} and those on the cross sections and the strength functions are very weak (less than 1 %). Only the effects on the polarization are significant.

We will assume a spherical spin-orbit coupling potential in the following discussion, because JUPITOR and ADAPE adopt the spherical approximation and because the effects on the cross sections are negligible.

II.4 Effect of number of coupled levels

The most interesting point is to know how many levels should be coupled. This must depend on the relation between the energy of the incident neutron and the energies of levels. Hence we examined this problem by doing the calculations with various couplings (up to 5 levels) at the energy of 0.1, 0.6 and 2 MeV. These energies are chosen so that i) in the first case (0.1 MeV) there are some subthreshold

levels, ii) in the second case (0.6 MeV) all the levels are open but are of the same order as the neutron energy, iii) in the last case (2 MeV) the neutron energy is much higher than the energies of the levels.

The results seem to converge with oscillations when the number of coupled levels increases. Therefore we take the results with coupling of 5 levels as standard values. The results are given in tables 5A, 5B and 5C for energies 0.1, 0.6 and 2 MeV respectively. The coupling of 1 level means that the potential is deformed but that no coupling is considered.

II.4.A - C matrix coefficients.

The differences of the diagonal C matrix coefficients from the standard values are given in tables 5A, 5B and 5C. Some of them are shown in figs.4A, 4B and 4C. The convergence with oscillations is very clear. The followings can be said on the diagonal coefficients ;

1) without coupling (coupling of 1 level), the results are very different from the other cases. The errors are of the order of 10^{-1} and of the same order as the errors due to the spherical approximations, though the potential is deformed in this case.

2) when 2 levels are coupled, the results are drastically improved. The errors become less than 5×10^{-2}.

3) with coupling of 3 levels, the errors are less than 10^{-2}.

4) with coupling of 4 levels, the errors become very small (less than 2×10^{-3}) and comparable with the errors due to the numerical integration.

At 0.1 MeV the absolute errors with coupling of 2 levels seem smaller than those at 0.6 and 2 MeV. This may be explained by the fact

that the third level of ^{238}U (4^+ ; E = 148 keV) is energetically closed. However, the relative errors are not always small, as the value of C matrix coefficients for p-wave is also small at this energy because of the centrifugal force.

The convergence of the off-diagonal C matrix coefficients is generally much slower than the diagonal coefficients. This should be kept in mind in the discussion on the elastic scattering.

II.4.B - Strength functions

The relative errors on the s-wave and p-wave strength functions are shown in fig.5. The p-wave strength function at 0.1 MeV has very large error (20 %) with coupling of 2 levels. This might seem inconsistent with the fact that the absolute errors in C matrix coefficients are small at 0.1 MeV. As we discussed previously, however, the relative errors of C matrix coefficients for p-wave are not small at this energy, because the value itself is also small. Without this exception, the relative errors are respectively less than 1 %, 5 % and 10 % with coupling of 4, 3 and 2 levels.

Without any coupling the s-wave strength function is smaller and p-wave strength function is greater at any energy.

II.4.C - Integrated cross sections

The reaction cross section and the elastic scattering cross section converge well with increasing number of coupled levels. The relative errors are respectively less than 0.5 %, 2 % and 10 % with coupling of 4, 3 and 2 levels.

As for inelastic scattering, a transition to the highest of the levels taken into account is always overestimated (about 50 %), because there is no competition with higher levels. This is also the case for the elastic scattering without coupling. The cross section to the second highest level is also overestimated (less than 20 %). This overestimation may be avoided by introducing the "fudge factor" for higher levels as the JUPITOR-code does. However this introduces new ambiguous parameters and causes another uncertainty on the results. The ECIS 70-code does not have this option.

II.4.D - Differential cross sections and polarizations

The differential cross sections and the polarizations of elastic scattering and inelastic scattering to the 2^+ and 4^+ state are shown in figs.6, 7A, 7B, 7C, 8A, 8B and 8C with the results calculated by the ADAPE-code.

The symbols used in these figures are as follows :

——	:	coupling of 5 levels
Δ	:	coupling of 4 levels
□	:	coupling of 3 levels
o	:	coupling of 2 levels
▽	:	coupling of 1 level (without coupling but with deformed potential)
—·—	:	spherical approximation
——	:	adiabatic approximation (calculated by ADAPE)

The relative deviations defined by eq.(1) are given in tables 5A, 5B and 5C.

If there is no coupling, the results are like those of the spherical approximation. At 0.1 MeV the curves with coupling of 1 level deviate even more than those with spherical approximation. Therefore the most important factor in the coupled channel calculation is not the deformation but the coupling of levels.

II.4.E - Time consideration

The CP running time is also given in tables 5A, 5B and 5C. The time for computation increases very rapidly with increasing number of coupled levels and with increasing maximum angular momentum. It should be noted that more memories are required for calculating the coupling of 5 levels.

II.4.F - Conclusion

Considering experimental errors and the time for computation, we can conclude as follows :

1) coupling of 2 levels might be enough for the reaction cross section, the integrated elastic scattering cross section and the strength function. The errors are less than 10 % for the cross sections and the s-wave strength function and less than 20 % for the p-wave strength function at low energy.

2) coupling of 3 levels should be used for calculating the differential elastic scattering cross section. If we need a precise p-wave strength function at low energy, this coupling should be taken. The errors in the integrated cross sections and the strength functions are less than 3 % with this coupling.

3) if we need the inelastic scattering cross section to the n-th level, a coupling up to the (n + 1)-th level is necessary. This needs a very long time for computation. In this case, the adiabatic approximation seems more convenient. We will discuss this problem in the next section.

II.5 Adiabatic approximation

The adiabatic approximation can be used if the energy of the incident particle is much higher than the energies of the ground-state rotational band and if we consider only couplings on the ground state rotational band. With this approximation, the coupling of all levels of the ground-state rotational band is considered automatically and therefore quite accurate results can be obtained. This approximation diminishes the number of coupled equations and saves the computing time.

We used the ADAPE code for this approximation. The JUPITOR code has also an option for the adiabatic approximation, but this option does not work with the Saclay version of the code. However, the results of ADAPE were compared with those of JUPITOR by Benzi [5] and the agreement was reported to be very good.

The results of ADAPE are compared with those of ECIS 70 (with coupling of 5 levels) in table 6. The differential cross sections are also given in figs.6, 7A, 7B, 7C, 8A and 8C with dashed lines. The agreements for the total and the elastic scattering cross sections are very good even at 0.1 MeV. As for the inelastic scattering cross sections to the 2^+ state, however, the disagreement increases with decreasing the incident energy. This suggests the failure of the adiabatic approximation in the low energies, because the results of ECIS 70 converge with coupling

of 5 levels. On the other hand, the disagreement exists even at 2 MeV in the inelastic scattering cross section to the 4^+ state. This can be explained by the fact that the inelastic scattering to the 4^+ state does not yet converge with coupling of 5 levels, as we can see from the figures.

The CP running time of ADAPE * is much shorter and same as the running time of ECIS 70 with coupling of 3 levels. Considering its short computing time and its theoretically accurate results for the inelastic scattering, the adiabatic approximation is very useful in the case where the energy of the incident neutron is higher than 1 MeV.

It is difficult to calculate the strength function with the adiabatic approximation. However this problem is not severe because the strength functions are required at low energies.

III - REASONABLE CONDITION FOR NUMERICAL CALCULATION

The errors due to the various physical approximations were found to be considerably large ; with coupling of 3 levels, for example, the error on the C matrix coefficients is less than 10^{-2}. On the other hand, the precision of C matrix coefficients is less than 10^{-3} with the present condition of numerical integration (mesh interval = 0.1 fm). Hence in order to save the computing time, we try to decrease the number of mesh points at the slight expense of the precision of the numerical integration.

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* see appendix 2

In order to find the optimal mesh interval, we calculate the case of 3 levels coupling at 0.6 MeV with changing the mesh interval (0.1, 0.3, 0.5, 0.75 and 1 fm). The results are given in table 7 and fig.9. The standard values are the results with 0.1 fm, and can be referred in table 4B. The computing time becomes half (40 sec to 20 sec) but the errors are still negligible with increasing the mesh interval to 0.3 fm (50 steps). With the mesh interval of 0.5 fm (30 steps) the computing time is further improved, but the error becomes significant in the inelastic scattering. With larger mesh interval, the error becomes very large.

The mesh interval of 0.3 fm (50 steps) can be recommended to be the most reasonable from this examination.

IV - EFFECT OF DEFORMATION PARAMETERS

The deformation parameters are the key parameters in the coupled channel calculation. The uncertainty on these values and the error caused by this uncertainty will be discussed in this section.

IV.1 Quadrupole deformation

The β_2-value is fairly well determined from the experiments, and is believed to be between 0.22 and 0.26 for ^{238}U. Here we examine the effect of this uncertainty. Assuming the coupling of 3 levels, we calculated three cases (with β_2 = 0.22, 0.24 and 0.28) at 0.6 and 2 MeV. The results are given in tables 8A and 8B and figs.10A and 10B. The case of β_2 = 0.24 is taken as the standard.

The errors caused by the uncertainty of ±8 % in β_2-value cannot be neglected. The absolute errors on the C matrix coefficients are less than 2×10^{-2}. The relative errors on the reaction cross sections and the elastic scattering cross sections are less than 2 % and the errors on the strength functions are less than 5 %. The errors on the inelastic scattering are much larger (up to 30 %).

It should be noted that the error due to the uncertainty in β_2-value are of the same order as those caused by assuming the coupling of 3 levels.

IV.2 Octupole deformation

The β_4-value is an open question. This is considered to be small and generally assumed to be zero in most of present calculations. The effects of this parameter are examined by doing calculations for various β_4-value (0, 0.05, 0.1 and 0.2) with the coupling of 3 levels. The same β_2-value (= 0.24) is used for all the cases. The results are given in tables 9A and 9B and in figs.11A and 11B. The standard is the case with $\beta_4 = 0$.

The effects are considerably large even with $\beta_4 = 0.05$. The errors on the C matrix coefficients reach 5×10^{-2}. The relative errors on the reaction cross section, the elastic scattering cross section and the strength functions are several percents. The effects on the inelastic scattering are much larger. The errors show some saturation or oscillation with increasing β_4-value.

The actual β_4-value might be smaller than 0.05, and it might be impossible that β_4-value is as much as 0.2. However, we must still keep it in mind that considerable errors can be caused by our neglecting β_4.

V - CONCLUSION

The analysis of nuclear data with the coupled channel optical model is a very complicated work. From various discussions in this report, we can recommend the optimal physical approximation and show the limit of possible errors.

As for the shape of the optical potential, we must consider the deformation of the imaginary potential as well as that of the real potential. The deformed potential should be expanded with Legendre polynomial at least up to $\lambda = 4$. We can neglect the deformation of the spin-orbit coupling potential, unless we are interested in a very precise polarization.

When the energy of the incident neutron is low (less than 1 MeV), the coupling of 3 levels seems most reasonable for calculating the reaction cross section, the elastic scattering cross section and the strength functions. If the inelastic scattering to the n-th state is required, the coupling to the (n+1)-th state is necessary. The errors with these conditions are less than 3 % for most of values. The error in the inelastic scattering to the n-th state is still about 20 %.

If the energy of the incident neutron is higher than 1 MeV, the adoption of the adiabatic approximation is highly recommended. More precise results especially for the inelastic scattering are obtained with much less computing time with this approximation.

In the coupled channel model, we must consider the contribution of neutrons with a high angular momentum which can be neglected in the spherical optical model (see appendix I).

The uncertainty of the deformation parameters causes considerable errors. The uncertainty of β_2-value is ± 10 % and that of β_4-value is a complete open question. Hence the errors due to these uncertainties are inevitable, even if the errors due to the physical approximations can be removed. The errors of the calculated results are estimated to be 3 % for the reaction and the elastic scattering cross sections, 5 % for the strength functions and 20 % for the inelastic scattering cross sections. We must keep these errors in mind in analyzing the nuclear data with the coupled channel optical model, whichever parameters of optical potential we may choose.

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Table 1

Optical model parameter and assumed level scheme

$$V(r) = V_R \times \frac{1}{1 + \exp\left(\frac{r - R_r}{a_r}\right)}$$

$$+ 4a_i W_S \left[-\frac{d}{dr} \frac{1}{1 + \exp\left(\frac{r - R_i}{a_i}\right)} \right]$$

$$+ \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{V_{SL}}{r} \left[-\frac{d}{dr} \frac{1}{1 + \exp\left(\frac{r - R_r}{a_r}\right)} \right] \vec{\ell} \cdot \vec{\sigma}$$

$$R_r = R_i = r_o A^{1/3} \left(1 + \sum_\lambda \beta_\lambda Y_{\lambda o}(\theta')\right)$$

V_R = 49.3 MeV
W_S = 5.75 MeV
V_{SL} = 5.5 MeV

r_o = 1.25 fm
a_r = 0.65 fm
a_i = 0.7 fm

β_2 = 0.24
β_4 = 0

} except section IV

Assumed levels of ^{238}U

I^π	Energy (MeV)
0^+	0
2^+	0.044
4^+	0.148
6^+	0.309
8^+	0.523

Table 2

Difference between deformed and spherical imaginary potential with coupling of 2 levels

Energy			0.6 MeV (J_{max} = 4.5)				2 MeV (J_{max} = 6.5)			
W_s			Deformed (standard)		spherical		Deformed (standard)		spherical	
σ_r	(mb)		4148		4175	(+0.65%)	4296		4363	(+1.6%)
σ_{el}	(mb)		4761		4957	(+4.1%)	3471		3523	(+1.5%)
$\sigma_{in(2^+)}$	(mb)		171.7		182.8	(+6.1%)	368.4		407.5	(+11%)
ξ_o	($\times 10^{-4}$)		1.256		1.279	(+1.8%)	0.890		0.930	(+4.4%)
ξ_1	($\times 10^{-4}$)		1.988		2.006	(+0.9%)	1.282		1.256	(-2.1%)
C_l^j			Value		Difference from standard		Value		Difference from standard	
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		-0.0562	0.8066	-0.0276	-0.0110	0.1849	0.3658	-0.0080	+0.0238
1	$1/2^-$		-0.2422	0.2675	-0.0117	+0.0249	-0.0722	0.5830	+0.0285	+0.0314
	$3/2^-$		-0.2119	0.2882	-0.0212	-0.0220	-0.0199	0.5683	+0.0157	+0.0369
2	$3/2^+$		-0.0653	0.0583	+0.0086	+0.0034	-0.2591	0.3892	+0.0275	-0.0131
	$5/2^+$		-0.0559	0.0626	+0.0079	-0.0008	-0.2504	0.3943	+0.0335	+0.0008
3	$5/2^-$		-0.0017	0.0064	+0.0009	+0.0008	-0.0660	0.1738	-0.0223	-0.0002
	$7/2^-$		-0.0012	0.0100	-0.0014	$<10^{-4}$	-0.1188	0.2195	-0.0109	-0.0175
4	$7/2^+$						-0.0056	0.0389	+0.0088	+0.0035
	$9/2^+$						-0.0101	0.0421	+0.0028	+0.0089
Relative dev.	Elastic	$\frac{d\sigma}{d\Omega}$			0.06				0.02	
		P			0.30				0.49	
	Inelas. (2^+)	$\frac{d\sigma}{d\Omega}$			0.16				0.13	
		P			0.50				0.39	
Time (sec.)			8.2		8.1		12		10	
Memory (K bytes)			245		245		245		245	

Table 3A

Effect of order of Legendre expansion at 0.6 MeV with coupling of 3 levels

Legendre expansion			P2		P4 (standard)		P6	
J_{max}			4.5		4.5		4.5	
σ_r	(mb)		3996	(-3.4%)	4137		4138	(+0.02%)
σ_{el}	(mb)		5475	(+3.5%)	5288		5283	(-0.09%)
$\sigma_{in(2^+)}$	(mb)		121.9	(-0.16%)	122.1		120.9	(-0.98%)
$\sigma_{in(4^+)}$	(mb)		8.52	(-7.2%)	9.18		9.26	(+0.87%)
ξ_o	($\times 10^{-4}$)		1.240	(-0.32%)	1.244		1.242	(-0.16%)
ξ_1	($\times 10^{-4}$)		1.878	(-6.2%)	2.004		2.009	(+0.25%)
$C_l^{J\pi}$			Difference from P4		Value		Difference from P4	
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		- 0.0123	- 0.0010	- 0.0399	0.8115	+ 0.0004	+ 0.0005
1	$1/2^-$		- 0.0221	+ 0.0092	- 0.2576	0.3209	+ 0.0007	- 0.0006
	$3/2^-$		- 0.0220	+ 0.0035	- 0.2488	0.3179	+ 0.0010	- 0.0002
2	$3/2^+$		+ 0.0034	- 0.0019	- 0.0706	0.0595	- 0.0002	- 0.0001
	$5/2^+$		+ 0.0050	- 0.0001	- 0.0679	0.0598	- 0.0002	- 0.0002
3	$5/2^-$		- 0.0010	$<10^{-4}$	- 0.0032	0.0079	$<10^{-4}$	$<10^{-4}$
	$7/2^-$		- 0.0009	- 0.0005	- 0.0031	0.0103	+ 0.0009	$<10^{-4}$
Relative deviation	Elastic	$\frac{d\sigma}{d\Omega}$	0.34				0.002	
		P	0.58				0.057	
	Inelastic (2^+)	$\frac{d\sigma}{d\Omega}$	0.008				0.010	
		P	0.14				0.010	
	Inelastic (4^+)	$\frac{d\sigma}{d\Omega}$	0.10				0.011	
		P	0.59				0.027	
Time (sec.)			38		42		41	
Memory (K bytes)			245		245		245	

Effect of order of Legendre expansion at 2 MeV
with coupling of 3 levels

Legendre expansion		P2		P4 (standard)		P6	
J_{max}		6.5		6.5		6.5	
σ_r	(mb)	4006	(-1.7%)	4013		4012	(-0.03%)
σ_{el}	(mb)	3695	(+2.0%)	3621		3617	(-0.11%)
$\sigma_{in(2^+)}$	(mb)	262.7	(+6.1%)	247.7		244.9	(-1.1%)
$\sigma_{in(4^+)}$	(mb)	63.46	(+2.0%)	62.20		62.73	(+0.85%)
ξ_o	($\times 10^{-4}$)	0.861	(+2.4%)	0.841		0.839	(-0.20%)
ξ_1	($\times 10^{-4}$)	1.218	(-2.6%)	1.250		1.250	(+0.06%)
C_l^j		Difference from P4		Value		Difference from P4	
l	J^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	- 0.0006	+ 0.0144	0.2009	0.3488	+ 0.0008	- 0.0002
1	$1/2^-$	+ 0.0037	+ 0.0305	- 0.0438	0.6291	- 0.0005	- 0.0147
	$3/2^-$	- 0.0055	- 0.0268	- 0.0185	0.6037	$<10^{-4}$	- 0.0007
2	$3/2^+$	+ 0.0113	- 0.0068	- 0.2812	0.3876	- 0.0005	- 0.0003
	$5/2^+$	+ 0.0161	- 0.0002	- 0.2730	0.3705	- 0.0004	- 0.0006
3	$5/2^-$	- 0.0112	- 0.0066	- 0.0913	0.1686	+ 0.0008	+ 0.0001
	$7/2^-$	- 0.0032	- 0.0106	- 0.1242	0.2039	+ 0.0002	+ 0.0006
4	$7/2^+$	+ 0.0032	+ 0.0021	- 0.0085	0.0327	- 0.0001	$<10^{-4}$
	$9/2^+$	+ 0.0004	+ 0.0040	- 0.0048	0.0377	$<10^{-4}$	- 0.0002
Relative deviation: Elastic	$\frac{d\sigma}{d\Omega}$	0.018				0.001	
	P	0.30				0.020	
Relative deviation: Inelastic (2^+)	$\frac{d\sigma}{d\Omega}$	0.075				0.011	
	P	0.11				0.096	
Relative deviation: Inelastic (4^+)	$\frac{d\sigma}{d\Omega}$	0.11				0.014	
	P	0.35				0.045	
Time (sec.)		64		73		69	
Memory (K bytes)		245		245		245	

Effect of deformed spin-orbit coupling force with coupling of 3 levels

Energy		0.6 MeV (J_{max} = 4.5)				2 MeV (J_{max} = 6.5)			
S-L force		Spherical (standard)		Deformed		Spherical (standard)		Deformed	
σ_r	(mb)	4137		4108	(-0.70%)	4013		4022	(+0.22%)
σ_{el}	(mb)	5288		5292	(+0.07%)	3622		3605	(-0.47%)
$\sigma_{in(2^+)}$	(mb)	122.1		120.9	(-0.98%)	247.6		247.3	(-0.12%)
$\sigma_{in(4^+)}$	(mb)	9.18		9.10	(-0.87%)	72.2		72.1	(-0.22%)
ξ_o	($\times 10^{-4}$)	1.244		1.243	(-0.08%)	0.841		0.840	(-0.11%)
ξ_1	($\times 10^{-4}$)	2.044		1.986	(-0.90%)	1.249		1.251	(+0.14%)
C_l^j		Value		Difference from standard		Value		Difference from standard	
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	-0.0399	0.8115	+0.0007	0.0004	0.2009	0.3487	+0.0016	+0.0001
1	$1/2^-$	-0.2576	0.3209	+0.0015	-0.0011	-0.0435	0.6293	-0.0007	-0.0073
	$3/2^-$	-0.2488	0.3179	-0.0035	-0.0015	-0.0183	0.6039	-0.0049	+0.0009
2	$3/2^+$	-0.0706	0.0595	-0.0003	-0.0010	-0.2812	0.3876	+0.0003	-0.0027
	$5/2^+$	-0.0679	0.0598	-0.0007	+0.0001	-0.2729	0.3705	-0.0007	-0.0006
3	$5/2^-$	-0.0032	0.0079	+0.0002	+0.0002	-0.0913	0.1686	+0.0015	+0.0053
	$7/2^-$	-0.0031	0.0103	+0.0001	-0.0003	-0.1241	0.2039	+0.0031	-0.0023
4	$7/2^+$					-0.0085	0.0327	+0.0010	-0.0010
	$9/2^+$					-0.0048	0.0377	-0.0010	+0.0007
Relative deviation: Elastic $\frac{d\sigma}{d\Omega}$ P				0.019				0.003	
				0.46				0.16	
Relative deviation: Inelastic (2^+) $\frac{d\sigma}{d\Omega}$ P				0.022				0.016	
				0.24				0.36	
Relative deviation: Inelastic (4^+) $\frac{d\sigma}{d\Omega}$ P				0.006				0.008	
				0.19				0.29	
Time (sec.)		42		44		73		72	
Memory (K bytes)		245		245		245		245	

Table 5_{A-1}

Effect of number of levels at 0.1 MeV (J_{max} = 4.5)

		5 Levels (standard)		4 levels		3 levels	
σ_r	(mb)	4874		4861 (-0.27%)		4963 (+1.8%)	
σ_{el}	(mb)	7776		7788 (+0.15%)		7779 (+0.04%)	
$\sigma_{in(2^+)}$	(mb)	9.57		9.61 (+0.41%)		9.67 (+1.04%)	
$\sigma_{in(4^+)}$	(mb)	0		0		0	
ξ_o	($\times 10^{-4}$)	1.576		1.567 (-0.6%)		1.613 (+2.4%)	
ξ_1	($\times 10^{-4}$)	3.006		3.002 (-0.2%)		3.043 (+1.2%)	
C_l^j		Value		Difference from standard value			
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	- 0.3903	0.3607	- 0.0006	+ 0.0002	+ 0.0021	+ 0.0009
1	$1/2^-$	- 0.0475	0.0369	$<10^{-4}$	- 0.0001	- 0.0041	+ 0.0008
	$3/2^-$	- 0.0486	0.0367	- 0.0006	- 0.0001	- 0.0022	+ 0.0007
2	$3/2^+$	- 0.0013	0.0012	$<10^{-4}$	+ 0.0001	$<10^{-4}$	+ 0.0001
	$5/2^+$	- 0.0012	0.0013	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
Relative dev. Elastic $\frac{d\sigma}{d\Omega}$				0.002		0.017	
	P			0.376		1.30	
Relative dev. Inelas. (2^+) $\frac{d\sigma}{d\Omega}$				0.007		0.042	
	P			0.084		0.568	
Time (sec.)		303		126		38	
Memory (K bytes)		401		245		245	

Table 5A-2

Effect of number of levels at 0.1 MeV (J_{max} = 4.5)

		2 levels		1 level		spherical	
σ_r	(mb)	4403	(-9.7%)	6582	(+35%)	6284	(+29%)
σ_{el}	(mb)	7552	(-2.9%)	8343	(+7.3%)	8164	(+5.0%)
$\sigma_{in(2^+)}$	(mb)	16.	(+67%)				
$\sigma_{in(4^+)}$	(mb)						
ξ_o	($\times 10^{-4}$)	1.544	(-2.0%)	0.938	(-41%)	0.839	(-47%)
ξ_1	($\times 10^{-4}$)	2.520	(-16%)	5.958	(+98%)	5.836	(+94%)

C_l^j		Difference from standard value					
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	+ 0.0005	- 0.0068	- 0.0275	- 0.0305	- 0.0319	- 0.0341
1	$1/2^-$	+ 0.0037	- 0.0094	- 0.0107	+ 0.0411	+ 0.0058	+ 0.0319
	$3/2^-$	- 0.0086	- 0.0049	- 0.0236	+ 0.0389	- 0.0063	+ 0.0369
2	$3/2^+$	+ 0.0001	$<10^{-4}$	+ 0.0001	- 0.0005	- 0.0001	- 0.0006
	$5/2^+$	+ 0.0002	$<10^{-4}$	+ 0.0002	- 0.0006	+ 0.0002	- 0.0007

Relative dev.					
Elastic	$\frac{d\sigma}{d\Omega}$	0.075	0.295	0.176
	P	7.21	11.2	3.49
Inelas. (2^+)	$\frac{d\sigma}{d\Omega}$	0.695		
	P	0.439		
Time (sec.)		7.3	~ 2	~ 2
Memory (K bytes)		245	245	245

Effect of number of levels at 0.6 MeV (J_{max} = 4.5)

		5 levels (standard)		4 levels		3 levels	
σ_r	(mb)	4144		4140 (-0.01%)		4137 (-0.17%)	
σ_{el}	(mb)	5225		5224 ($<10^{-2}$%)		5288 (+1.2%)	
$\sigma_{in(2^+)}$	(mb)	106.6		103.6 (-2.8%)		122.1 (+15%)	
$\sigma_{in(4^+)}$	(mb)	6.51		6.72 (3.2%)		9.18 (+41%)	
ξ_o	($\times 10^{-4}$)	1.220		1.212 (+0.7%)		1.244 (+2.1%)	
ξ_1	($\times 10^{-4}$)	2.043		2.048 (+0.9%)		2.004 (-1.9%)	
C_l^j		Value		Difference from standard value			
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	- 0.0445	0.8156	- 0.0004	+ 0.0015	+ 0.0106	- 0.0041
1	$1/2^-$	- 0.2451	0.3162	+ 0.0001	- 0.0009	- 0.0125	+ 0.0047
	$3/2^-$	- 0.2421	0.3148	+ 0.0017	- 0.0002	- 0.0067	+ 0.0031
2	$3/2^+$	- 0.0701	0.0575	- 0.0004	- 0.0001	- 0.0005	+ 0.0020
	$5/2^+$	- 0.0658	0.0592	+ 0.0001	- 0.0004	- 0.0021	+ 0.0006
3	$5/2^-$	- 0.0027	0.0077	$<10^{-4}$	$<10^{-4}$	- 0.0005	+ 0.0002
	$7/2^-$	- 0.0027	0.0104	+ 0.0002	$<10^{-4}$	- 0.0004	- 0.0001
Relative deviation	Elastic $\frac{d\sigma}{d\Omega}$ P			0.002 0.22		0.020 0.98	
	Inelastic (2^+) $\frac{d\sigma}{d\Omega}$ P			0.029 0.019		0.15 0.35	
	Inelastic (4^+) $\frac{d\sigma}{d\Omega}$ P			0.025 0.88		0.41 1.77	
Time (sec.)		317		133		42	
Memory (K bytes)		401		245		245	

Effect of number of levels at 0.6 MeV (J_{max} = 4.5)

			2 levels		1 level		spherical	
σ_r	(mb)		4148	(+0.01%)	4263	(2.9%)	4201	(1.4%)
σ_{el}	(mb)		4761	(-8.9%)	7307	(40%)	6737	(37%)
$\sigma_{in(2^+)}$	(mb)		171.7	(61%)				
$\sigma_{in(4^+)}$	(mb)							
ξ_0	($\times 10^{-4}$)		1.256	(+30%)	0.815	(-33%)	0.734	(-40%)
ξ_1	($\times 10^{-4}$)		1.988	(-2.7%)	2.543	(+24%)	2.708	(+32%)
C_l^j			Difference from standard value					
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		- 0.0117	- 0.0090	- 0.0635	+ 0.0576	- 0.0689	+ 0.0690
1	$1/2^-$		+ 0.0029	- 0.0487	+ 0.0396	+ 0.1536	+ 0.0710	+ 0.1058
	$3/2^-$		+ 0.0302	- 0.0266	- 0.0038	+ 0.1707	+ 0.0332	+ 0.1384
2	$3/2^+$		+ 0.0048	+ 0.0008	+ 0.0074	- 0.0218	+ 0.0062	+ 0.0269
	$5/2^+$		+ 0.0099	+ 0.0034	+ 0.0134	- 0.0216	+ 0.0111	- 0.0276
3	$5/2^-$		+ 0.0010	- 0.0013	+ 0.0003	+ 0.0107	+ 0.0017	+ 0.0070
	$7/2^-$		+ 0.0015	+ 0.0052	- 0.0087	+ 0.0058	- 0.0057	+ 0.0052
Relative deviation	Elastic	$\frac{d\sigma}{d\Omega}$	0.10		0.43		0.29	
		P	3.34		9.53		11.3	
	Inelastic (2^+)	$\frac{d\sigma}{d\Omega}$	0.67					
		P	0.32					
	Inelastic (4^+)	$\frac{d\sigma}{d\Omega}$						
		P						
Time (sec.)			8.2		1.6		~2	
Memory (K bytes)			245		245		245	

Table 5C-1

Effect of number of levels at 2 MeV (J_{max} = 6.5)

		5 levels (standard)		4 levels		3 levels	
σ_r	(mb)	4072		4075	(+0.07%)	4013	(-1.5%)
σ_{el}	(mb)	3586		3579	(-0.2%)	3621	(+0.98%)
$\sigma_{in(2^+)}$	(mb)	233.6		225.7	(-3.4%)	247.7	(6%)
$\sigma_{in(4^+)}$	(mb)	43.04		46.38	(+7.8%)	62.20	(45%)
ξ_o	($\times 10^{-4}$)	0.852		0.853	(+0.07%)	0.841	(-1.3%)
ξ_1	($\times 10^{-4}$)	1.257		1.257	(+0.05%)	1.250	(-0.6%)
C_l^j		Value		Difference from standard value			
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	+ 0.2021	0.3591	+ 0.0009	+ 0.0010	- 0.0012	- 0.0103
1	$1/2^-$	- 0.0392	0.6226	+ 0.0002	- 0.0010	- 0.0046	+ 0.0065
	$3/2^-$	- 0.0168	0.5990	+ 0.0008	- 0.0002	- 0.0017	+ 0.0047
2	$3/2^+$	- 0.2761	0.3807	- 0.0006	- 0.0015	- 0.0051	+ 0.0069
	$5/2^+$	- 0.2652	0.3735	+ 0.0018	- 0.0008	- 0.0078	- 0.0030
3	$5/2^-$	- 0.0879	0.1721	- 0.0002	+ 0.0005	- 0.0034	- 0.0035
	$7/2^-$	- 0.1253	0.2065	- 0.0005	+ 0.0004	+ 0.0011	- 0.0026
4	$7/2^+$	- 0.0070	0.0328	+ 0.0001	- 0.0002	- 0.0015	- 0.0001
	$9/2^+$	- 0.0051	0.0391	+ 0.0003	+ 0.0001	+ 0.0003	- 0.0014
Relative deviation: Elastic	$\frac{d\sigma}{d\Omega}$ P			0.002 0.045		0.003 0.15	
Relative deviation: Inelastic (2^+)	$\frac{d\sigma}{d\Omega}$ P			0.033 0.14		0.067 0.13	
Relative deviation: Inelastic (4^+)	$\frac{d\sigma}{d\Omega}$ P			0.079 0.63		0.40 0.78	
Time (sec.)		746		285		73	
Memory (K bytes)		401		245		245	

Table 5C-2

Effect of number of levels at 2 MeV (J_{max} = 6.5)

		2 levels		1 level		Spherical	
σ_r	(mb)	4295	(+5.5%)	3822	(-6.1%)	3424	(-16%)
σ_{el}	(mb)	3471	(-3.2%)	3540	(-1.8%)	3629	(-12%)
$\sigma_{in(2^+)}$	(mb)	368.4	(+58%)				
$\sigma_{in(4^+)}$	(mb)						
ξ_o	($\times 10^{-4}$)	0.890	(+4.5%)	0.683	(-20%)	0.617	(-28%)
ξ_1	($\times 10^{-4}$)	1.282	(+2.0%)	1.091	(-13%)	1.176	(-6.4%)

C_l^j		Difference from standard value					
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	- 0.0172	+ 0.0067	+ 0.0971	+ 0.0475	+ 0.1174	+ 0.0364
1	$1/2^-$	- 0.0330	- 0.0396	+ 0.2021	- 0.0430	+ 0.1566	- 0.0627
	$3/2^-$	- 0.0031	- 0.0307	+ 0.2008	+ 0.0242	+ 0.1664	+ 0.0015
2	$3/2^+$	+ 0.0017	+ 0.0035	- 0.0096	- 0.0845	- 0.0326	- 0.0935
	$5/2^+$	+ 0.0148	+ 0.0208	+ 0.0210	- 0.0931	- 0.0067	- 0.1047
3	$5/2^-$	+ 0.0219	+ 0.0117	- 0.1019	+ 0.0849	- 0.0714	+ 0.0756
	$7/2^-$	+ 0.0065	+ 0.0130	- 0.0980	- 0.0107	- 0.0828	- 0.0098
4	$7/2^+$	+ 0.0014	+ 0.0061	+ 0.0130	- 0.0077	+ 0.0053	- 0.0137
	$9/2^+$	- 0.0050	+ 0.0030	+ 0.0222	- 0.0028	- 0.0174	- 0.0117

Relative deviation			2 levels	1 level	Spherical
Elastic	$\frac{d\sigma}{d\Omega}$		0.016	0.11	0.16
	P		0.40	1.80	1.71
Inelastic	(2^+)	$\frac{d\sigma}{d\Omega}$	0.57		
		P	0.72		
	(4^+)	$\frac{d\sigma}{d\Omega}$			
		P			
Time (sec.)			12	1.6	2.1
Memory (K bytes)			245	245	245

Table 6

Comparison between the results of ADAPE and those of ECIS70

with coupling of 5 levels

Energy (MeV)				0.1		0.6		2	
Code				ADAPE	ECIS70	ADAPE	ECIS70	ADAPE	ECIS70
				l_{max}=9	J_{max}=4.5	l_{max}=9	J_{max}=4.5	l_{max}=12	J_{max}=6.5
σ_{el} (mb)				7782	7776 (-0.1%)	5230	5225 (-0.1%)	3583	3586 (+0.1%)
$\sigma_{in(2^+)}$ (mb)				19.4	9.6(-50%)	113.6	106.6(-6.2%)	237.6	233.6(-1.7%)
$\sigma_{in(4^+)}$ (mb)						10.1	6.5(-36%)	47.4	43.0(-9.3%)
σ_T (mb)				12651	12650 (-0.01%)	9359	9369 (+0.1%)	7651	7658 (+0.1%)
Relative deviation	Elastic		$\frac{d\sigma}{d\Omega}$	0.001		0.002		0.002	
	Inelastic	(2^+)	$\frac{d\sigma}{d\Omega}$	1.03		0.061		0.018	
		(4^+)	$\frac{d\sigma}{d\Omega}$			0.51		0.10	
Time (sec.)				46	303	50	316	98	746
Memory (K bytes)				180	245	180	245	180	245

Table 7

Effect of mesh interval at 0.6 MeV

with coupling of 3 levels (J_{max} = 4.5)

Mesh interval (fm)			0.3		0.5		0.75		1.0	
σ_r	(mb)		4137	(<0.02%)	4135	(-0.05%)	4125	(-0.3%)	4096	(-1.0%)
σ_{el}	(mb)		5290	(+0.04%)	5298	(+0.19%)	5326	(+0.7%)	5388	(+1.4%)
$\sigma_{in(2^+)}$	(mb)		121.9	(-0.16%)	121.2	(-0.74%)	118.8	(-2.7%)	112.7	(-7.7%)
$\sigma_{in(4^+)}$	(mb)		9.18	(<0.05%)	9.17	(-0.11%)	9.08	(-1.1%)	8.73	(-4.9%)
ξ_o	($\times 10^{-4}$)		1.244	(-0.04%)	1.241	(-0.30%)	1.227	(-1.5%)	1.186	(-4.6%)
ξ_1	($\times 10^{-4}$)		2.003	(-0.05%)	2.004	(<0.05%)	2.003	(-0.05%)	2.004	(<0.05%)
C_l^j			Difference from the value with mesh interval of 0.1 fm							
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		$<10^{-4}$	+0.0001	+0.0004	+0.0007	+0.0024	+0.0037	+0.0002	+0.0122
1	$1/2^-$		-0.0001	-0.0001	-0.0003	+0.0004	-0.0008	+0.0010	+0.0008	+0.0019
	$3/2^-$		-0.0001	+0.0001	-0.0003	+0.0003	-0.0009	+0.0008	-0.0012	+0.0012
2	$3/2^+$		$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	+0.0002	-0.0002	+0.0006	-0.0007
	$5/2^+$		$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	+0.0003	-0.0001	+0.0010	-0.0007
3	$5/2^-$		$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
	$7/2^-$		$<10^{-4}$	$<10^{-4}$	+0.0001	$<10^{-4}$	+0.0001	$<10^{-4}$	+0.0001	$<10^{-4}$
Relative dev.	Elastic	$\frac{d\sigma}{d\Omega}$	0.0003		0.0015		0.005		0.010	
		P	0.0014		0.006		0.019		0.047	
	Inelas.	(2^+) $\frac{d\sigma}{d\Omega}$	0.002		0.008		0.032		0.097	
		P	0.003		0.012		0.052		0.191	
Time (sec.)			20		16		11		10	
Memory (K bytes)			245		245		245		245	

Table 8-A

Effect of β_2-value at 0.6 MeV with coupling of 3 levels (J_{max} = 4.5)

β_2		0.22		0.24 (standard)		0.26	
σ_r	(mb)	4140	(+0.07%)	4137		4093	(-1.1%)
σ_{el}	(mb)	5346	(+1.1%)	5288		5276	(-0.2%)
$\sigma_{in(2^+)}$	(mb)	118.6	(-2.9%)	122.1		120.7	(+1.7%)
$\sigma_{in(4^+)}$	(mb)	7.12	(-22%)	9.18		11.3	(+23%)
ξ_o	($\times 10^{-4}$)	1.192	(-4.2%)	1.244		1.269	(+2.0%)
ξ_1	($\times 10^{-4}$)	2.087	(+4.2%)	2.004		1.924	(-4.0%)

C_1^j			Difference from standard		Value		Difference from standard	
1		j^π	Real	Imag.	Real	Imag.	Real	Imag.
0		$1/2^+$	- 0.0198	+ 0.0072	- 0.0399	0.8115	+ 0.0196	- 0.0029
1		$1/2^-$	+ 0.0077	+ 0.0055	- 0.2576	0.3209	- 0.0075	- 0.0048
		$3/2^-$	+ 0.0068	+ 0.0090	- 0.2488	0.3179	- 0.0068	- 0.0080
2		$3/2^+$	+ 0.0036	- 0.0050	- 0.0706	0.0595	- 0.0050	+ 0.0042
		$5/2^+$	+ 0.0053	- 0.0032	- 0.0679	0.0598	- 0.0059	+ 0.0016
3		$5/2^-$	+ 0.0001	+ 0.0004	- 0.0032	0.0079	- 0.0001	- 0.0003
		$7/2^-$	- 0.0002	+ 0.0004	- 0.0031	0.0103	+ 0.0002	- 0.0004
4		$7/2^+$						
		$9/2^+$						
Relative deviation	Elastic	$\frac{d\sigma}{d\Omega}$	0.013				0.010	
		P	0.33				0.15	
	Inelastic (2^+)	$\frac{d\sigma}{d\Omega}$	0.059				0.089	
		P	0.17				0.13	
	Inelastic (4^+)	$\frac{d\sigma}{d\Omega}$	0.24				0.24	
		P	0.24				0.19	

Table 8-B

Effect of β_2-value at 2 MeV with coupling of 3 levels (J_{max} = 6.5)

β_2			0.22		0.24 (standard)		0.26	
σ_r	(mb)		4034	(+0.5%)	4013		3973	(-1.0%)
σ_{el}	(mb)		3554	(-1.9%)	3622		3693	(+2.0%)
$\sigma_{in(2^+)}$	(mb)		248.0	(+0.2%)	247.7		239.3	(-3.4%)
$\sigma_{in(4^+)}$	(mb)		49.96	(-20%)	62.20		74.36	(+20%)
ξ_o	($\times 10^{-4}$)		0.835	(-0.7%)	0.841		0.842	(+0.1%)
ξ_1	($\times 10^{-4}$)		1.260	(+0.9%)	1.250		1.234	(-1.2%)
C_1^j			Difference from standard		Value		Difference from standard	
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		+ 0.0117	+ 0.0123	+ 0.2009	0.3488	- 0.0019	- 0.0117
1	$1/2^-$		+ 0.0144	- 0.0109	- 0.0438	0.6291	- 0.0133	+ 0.0108
	$3/2^-$		+ 0.0189	- 0.0047	- 0.0185	0.6037	- 0.0183	+ 0.0056
2	$3/2^+$		+ 0.0045	- 0.0154	- 0.2812	0.3870	- 0.0066	+ 0.0130
	$5/2^+$		+ 0.0072	- 0.0097	- 0.2730	0.3705	- 0.0067	+ 0.0077
3	$5/2^-$		- 0.0032	+ 0.0075	- 0.0913	0.1686	+ 0.0025	- 0.0069
	$7/2^-$		- 0.0098	+ 0.0023	- 0.1241	0.2039	+ 0.0093	- 0.0027
4	$7/2^+$		+ 0.0028	- 0.0004	- 0.0085	0.0327	- 0.0024	$<10^{-4}$
	$9/2^+$		+ 0.0023	+ 0.0006	- 0.0048	0.0377	- 0.0018	- 0.0008
Relative deviation	Elastic	$\frac{d\sigma}{d\Omega}$	0.020				0.017	
		P	0.14				0.13	
	Inelastic (2^+)	$\frac{d\sigma}{d\Omega}$	0.20				0.37	
		P	0.17				0.17	
	Inelastic (4^+)	$\frac{d\sigma}{d\Omega}$	0.21				0.22	
		P	0.10				0.11	

Table 9-A

Effect of β_4-value at 0.6 MeV with coupling of 3 levels

($\beta_2 = 0.24$, $J_{max} = 4.5$)

β_4		0 (standard)	0.05		0.1		0.2	
σ_r	(mb)	4137	4023	(-2.8%)	3856	(-6.8%)	3970	(-4.0%)
σ_{el}	(mb)	5288	5297	(+0.2%)	5365	(+1.5%)	5357	(+1.3%)
$\sigma_{in(2^+)}$	(mb)	122.1	104.8	(-14%)	89.1	(-27%)	136.6	(+12%)
$\sigma_{in(4^+)}$	(mb)	9.18	13.17	(+43%)	13.84	(+51%)	10.77	(+17%)
ξ_o	($\times 10^{-4}$)	1.244	1.213	(-2.5%)	1.148	(-7.7%)	1.258	(+1.1%)
ξ_1	($\times 10^{-4}$)	2.004	1.947	(-2.8%)	1.910	(-4.7%)	1.894	(-5.5%)

C_l^j		Value		Difference from standard					
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	-0.0399	0.8115	+0.0406	+0.0086	+0.0204	+0.0200	+0.0165	-0.0010
1	$1/2^-$	-0.2576	0.3209	+0.0033	-0.0091	+0.0060	-0.0140	+0.0026	-0.0050
	$3/2^-$	-0.2488	0.3179	-0.0021	-0.0127	-0.0052	-0.0188	-0.0172	-0.0097
2	$3/2^+$	-0.0706	0.0595	-0.0158	+0.0047	-0.0228	+0.0031	-0.0202	+0.0054
	$5/2^+$	-0.0679	0.0598	-0.0133	-0.0015	-0.0202	-0.0055	-0.0223	-0.0034
3	$5/2^-$	-0.0032	0.0019	+0.0003	-0.0003	+0.0005	-0.0002	+0.0004	+0.0015
	$7/2^-$	-0.0031	0.0103	+0.0011	-0.0005	+0.0018	-0.0009	+0.0017	-0.0004
4	$7/2^+$								
	$9/2^+$								

Relative deviation						
Elastic	$\frac{d\sigma}{d\Omega}$			0.019	0.030	0.022
	P			1.04	1.81	2.22
Inelastic	(2^+)	$\frac{d\sigma}{d\Omega}$		0.29	0.56	0.69
		P		0.33	0.59	0.73
	(4^+)	$\frac{d\sigma}{d\Omega}$		0.43	0.49	0.18
		P		0.98	1.18	1.15

Table 9-B

Effect of β_4-value at 2 MeV with coupling of 3 levels

($\beta_2 = 0.24$, $J_{max} = 6.5$)

β_4			0 (standard)		0.05		0.1		0.2	
σ_r	(mb)		4013		3891	(-3.0%)	3789	(-5.6%)	3810	(-5.1%)
σ_{el}	(mb)		3622		3718	(+2.7%)	3799	(+4.9%)	3942	(+8.8%)
$\sigma_{in(2^+)}$	(mb)		247.7		205.2	(-17%)	167.1	(-33%)	228.6	(-7.7%)
$\sigma_{in(4^+)}$	(mb)		62.20		83.73	(+35%)	96.27	(+55%)	95.92	(+54%)
ξ_o	($\times 10^{-4}$)		0.841		0.788	(-6.3%)	0.780	(-7.3%)	0.808	(-3.9%)
ξ_1	($\times 10^{-4}$)		1.250		1.236	(-1.1%)	1.214	(-2.9%)	1.179	(-5.7%)
C_l^j			Value		Difference from standard					
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		+0.2009	0.3488	-0.0099	-0.0347	-0.0178	-0.0569	-0.0463	-0.0645
1	$1/2^-$		-0.0438	0.6291	-0.0246	+0.0032	-0.0429	+0.0045	-0.0521	+0.0068
	$3/2^-$		-0.0185	0.6037	-0.0375	-0.0037	-0.0699	-0.0035	-0.0999	+0.0078
2	$3/2^+$		-0.2812	0.3870	-0.0266	+0.0224	-0.0440	+0.0327	-0.0413	+0.0437
	$5/2^+$		-0.2730	0.3705	-0.0252	+0.0105	-0.0410	+0.0174	-0.0047	+0.0343
3	$5/2^-$		-0.0913	0.1686	+0.0092	-0.0100	+0.0136	-0.0150	+0.0023	-0.0050
	$7/2^-$		-0.1241	0.2039	+0.0236	+0.0020	+0.0444	+0.0024	+0.0551	+0.0022
4	$7/2^+$		-0.0085	0.0327	-0.0055	-0.0033	-0.0082	-0.0067	-0.0087	-0.0091
	$9/2^+$		-0.0048	0.0377	-0.0037	-0.0042	-0.0057	-0.0074	-0.0068	-0.0094
Relative deviation	Elastic	$\frac{d\sigma}{d\Omega}$ P			0.016		0.028		0.077	
					0.27		0.49		0.80	
	Inelastic	(2^+) $\frac{d\sigma}{d\Omega}$ P			0.18		0.34		0.26	
					0.37		0.60		1.40	
		(4^+) $\frac{d\sigma}{d\Omega}$ P			0.40		0.64		0.60	
					0.36		0.70		0.95	

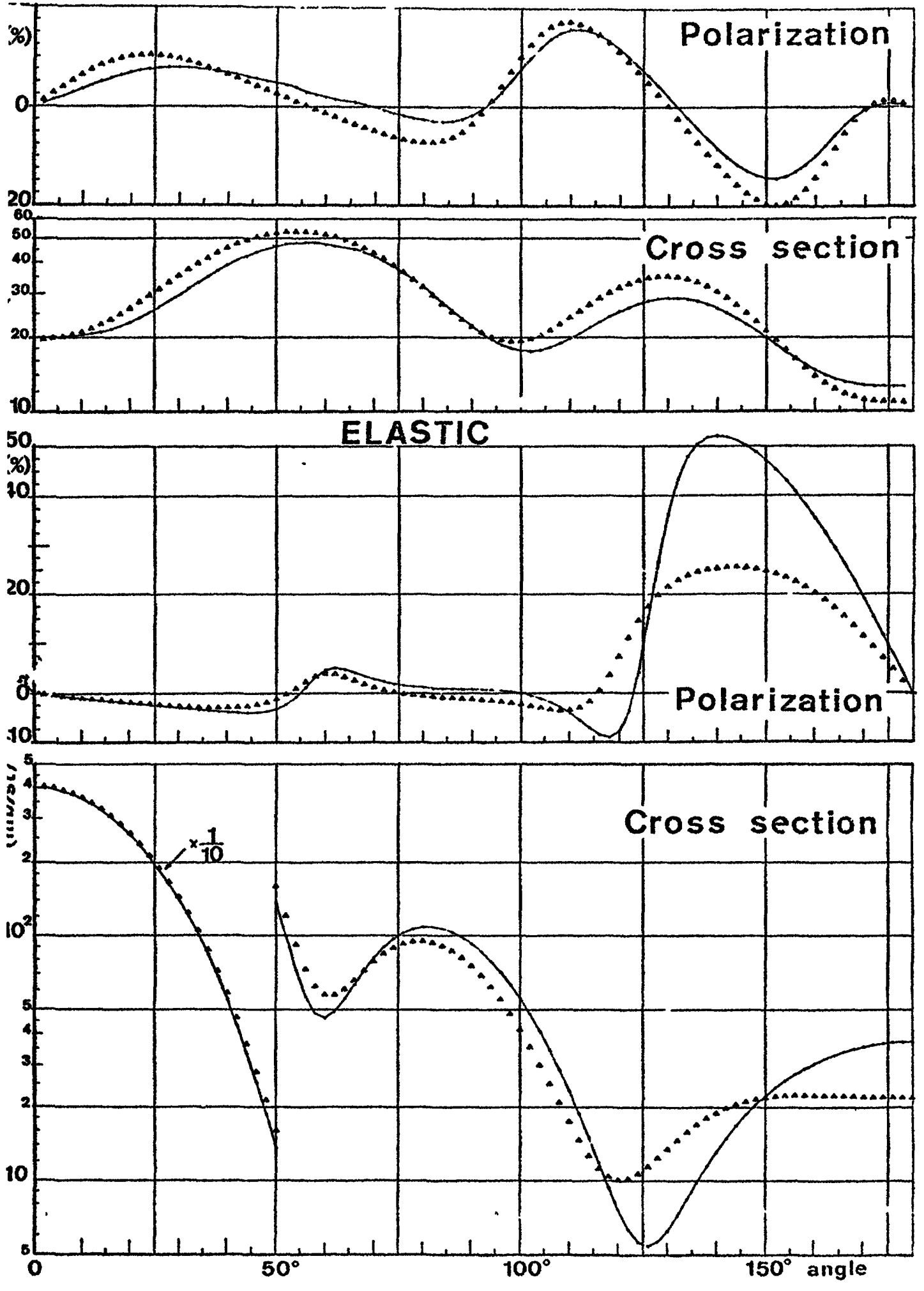

Fig. 1 Effect of the deformation of the imaginary potential at 2 MeV

(— · deformed w Δ · sperical) w

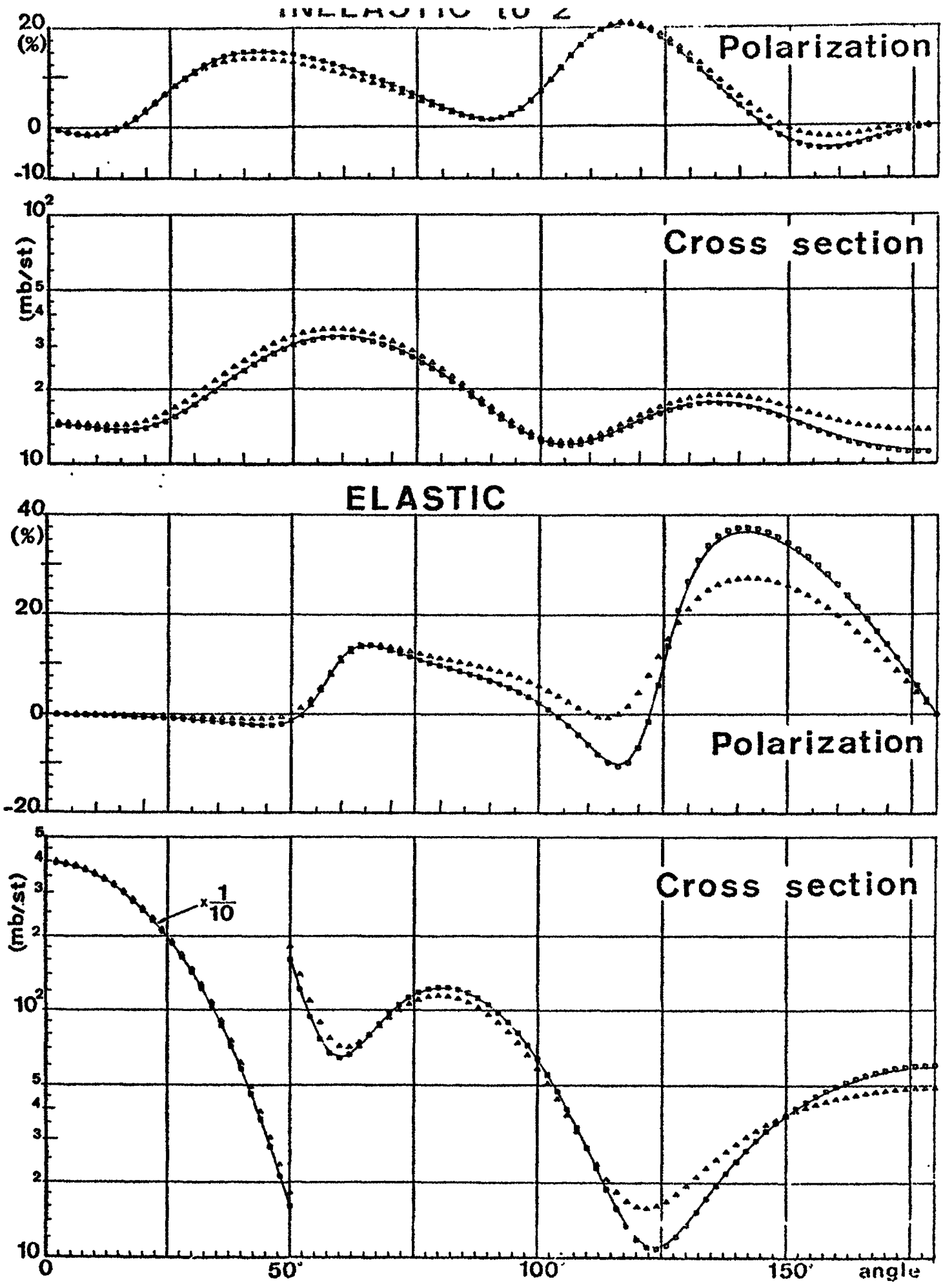

Fig. 2 Effect of Order of Legendre Expansion at 2 MeV

(— : P4 expansion, ▲ : P2 expansion, □ : P6 expansion)

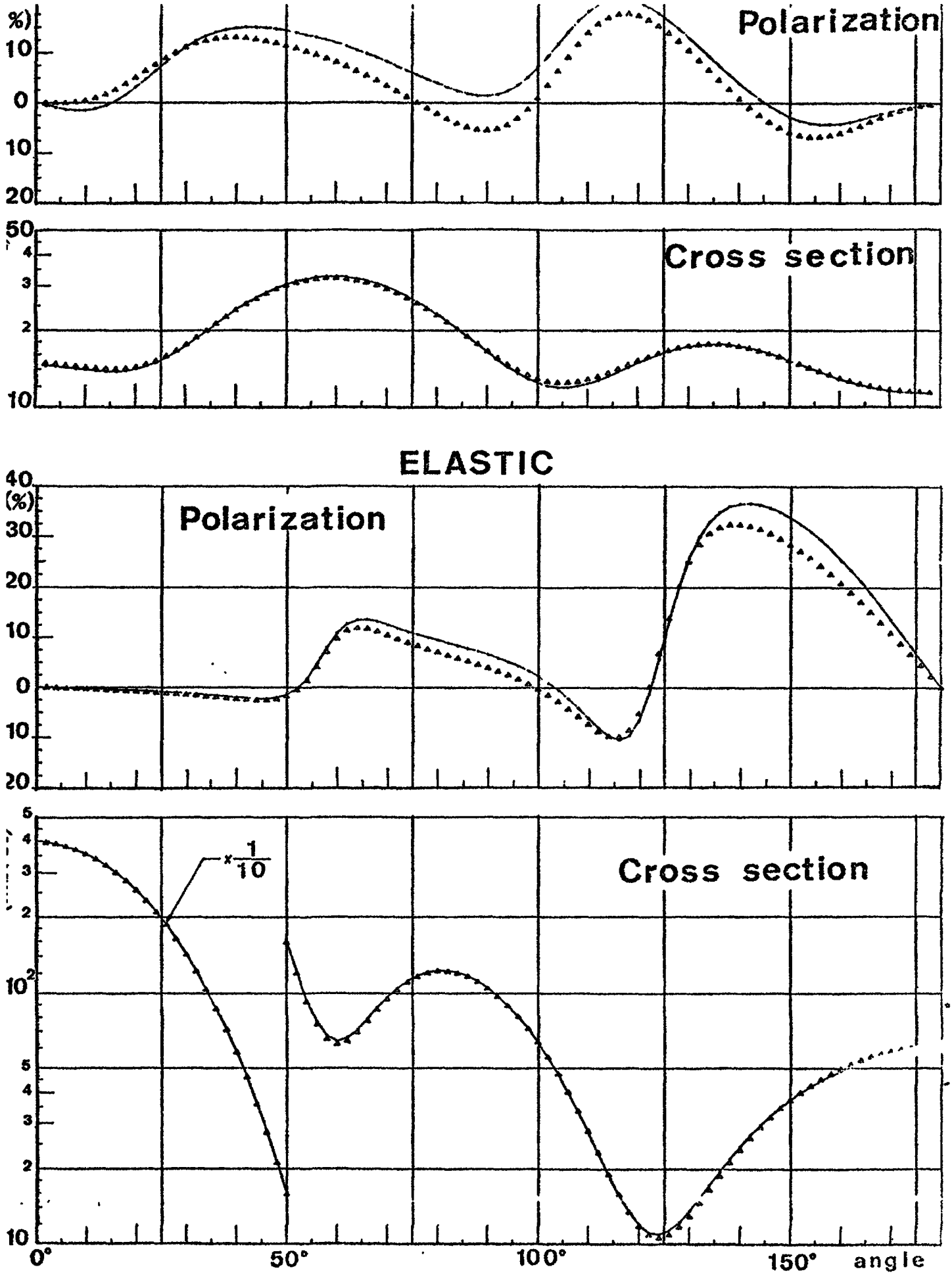

Fig. 3 Effect of Deformation of Spin-Orbit Coupling Potential

(— : spherical V_{SL} , Δ: deformed V_{SL} .)

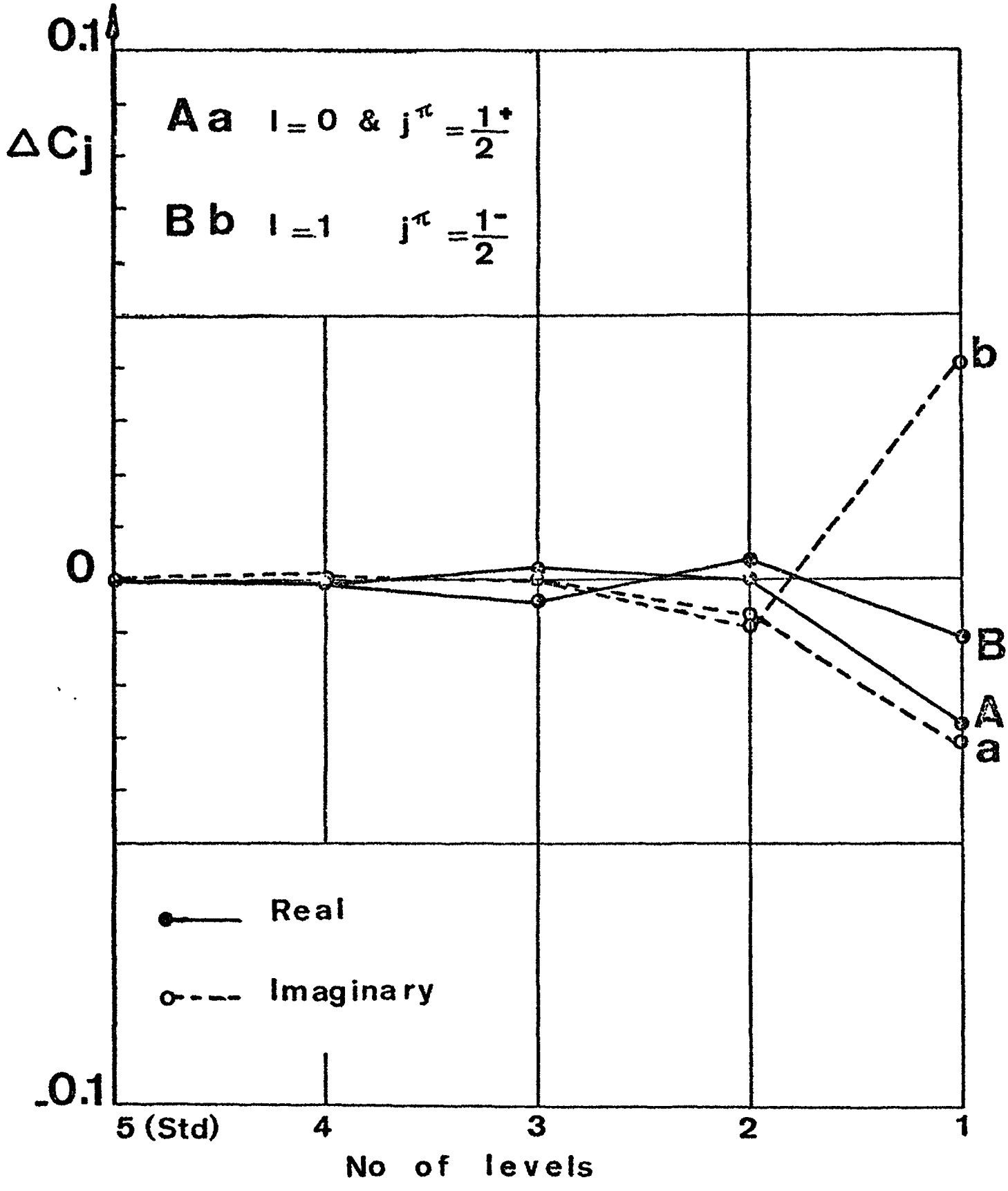

Fig. 4 A The absolute errors of some diagonal C-matrix coefficients at 0.1 MeV with various couplings

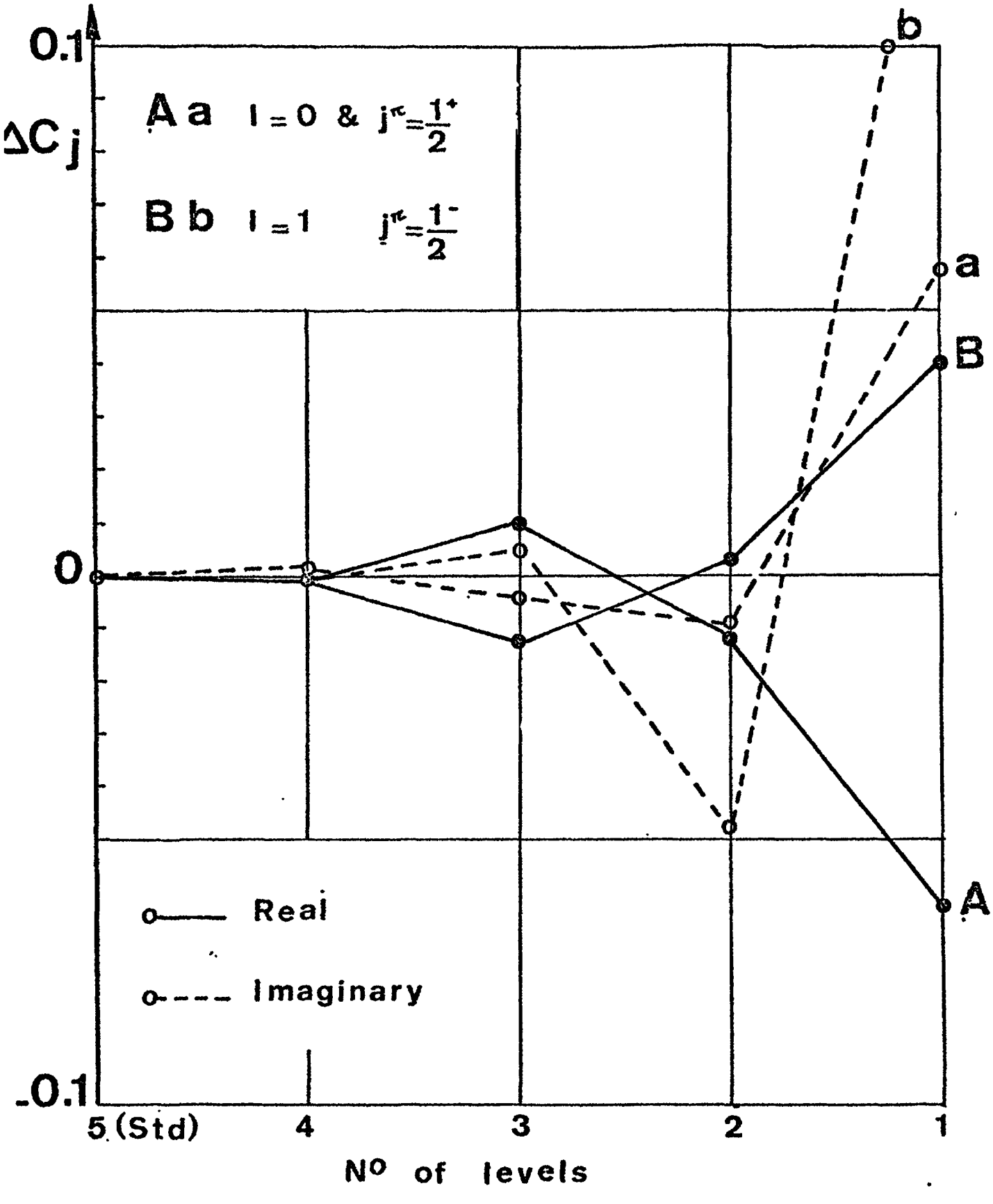

Fig. 4 B The absolute errors of some diagonal C-matrix coefficients at 0.6 MeV with various couplings

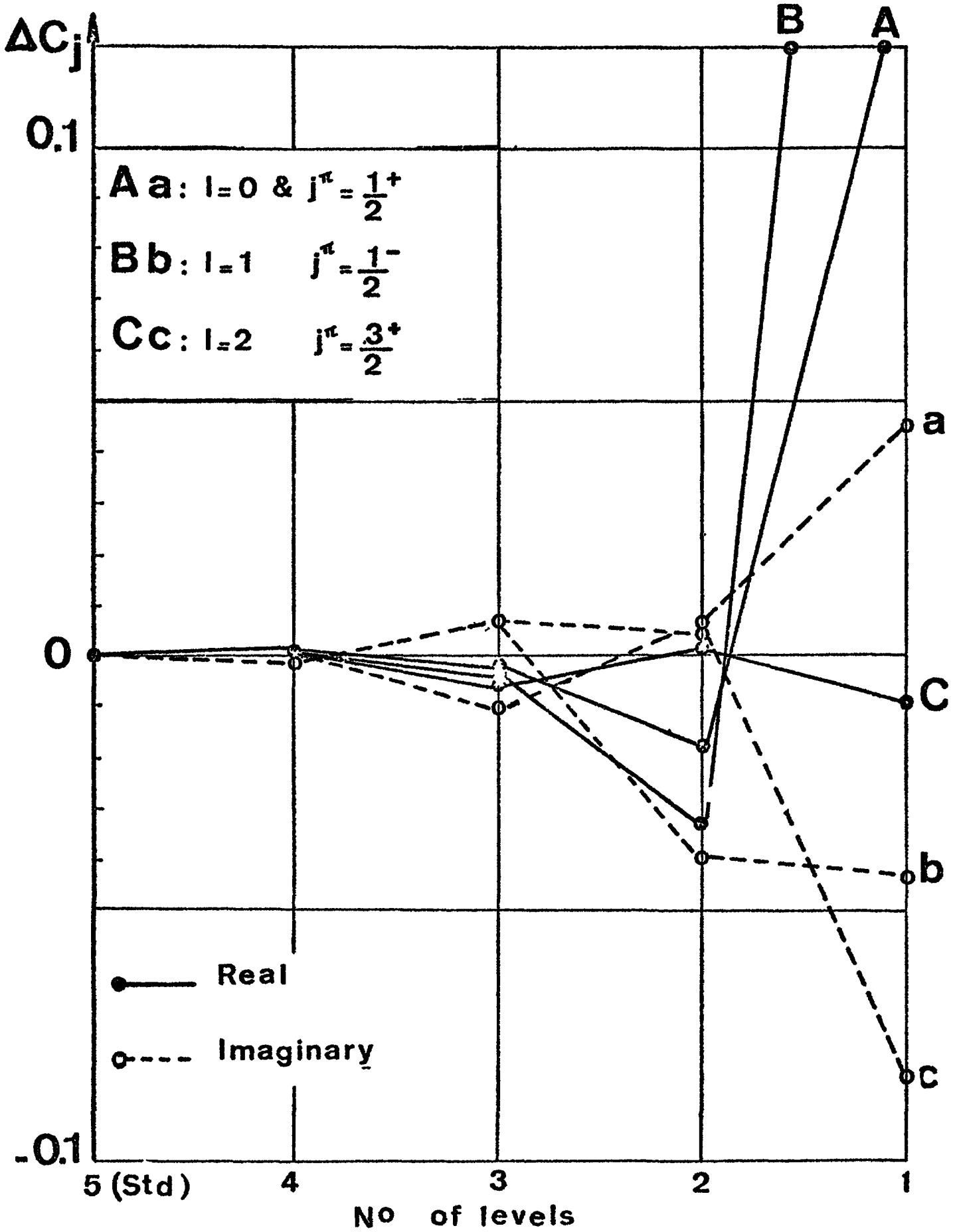

Fig. 4 C The absolute errors of some diagonal C-matrix coefficients at 2 MeV with various couplings

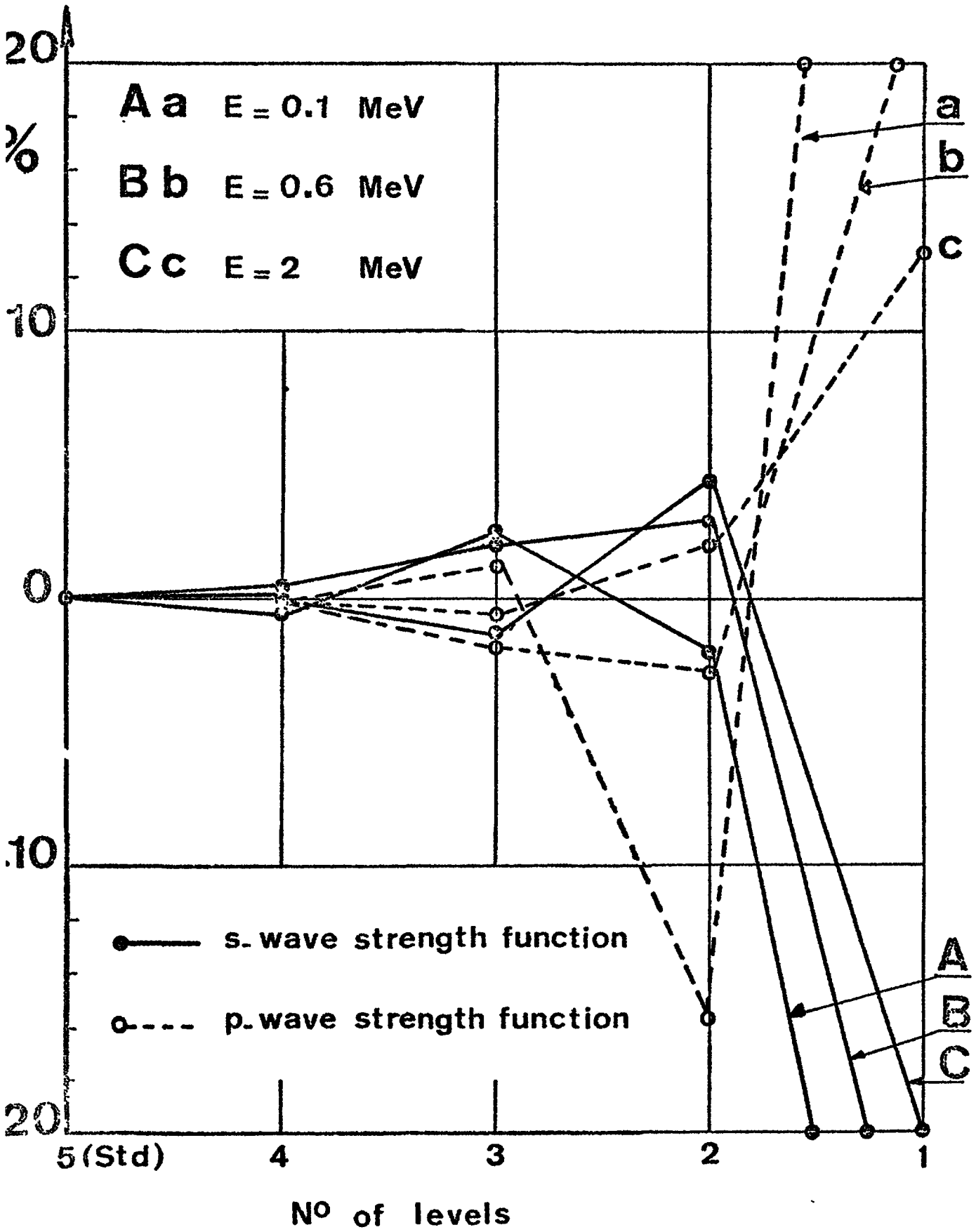

Fig. 5 The relative errors of the strength functions with various couplings

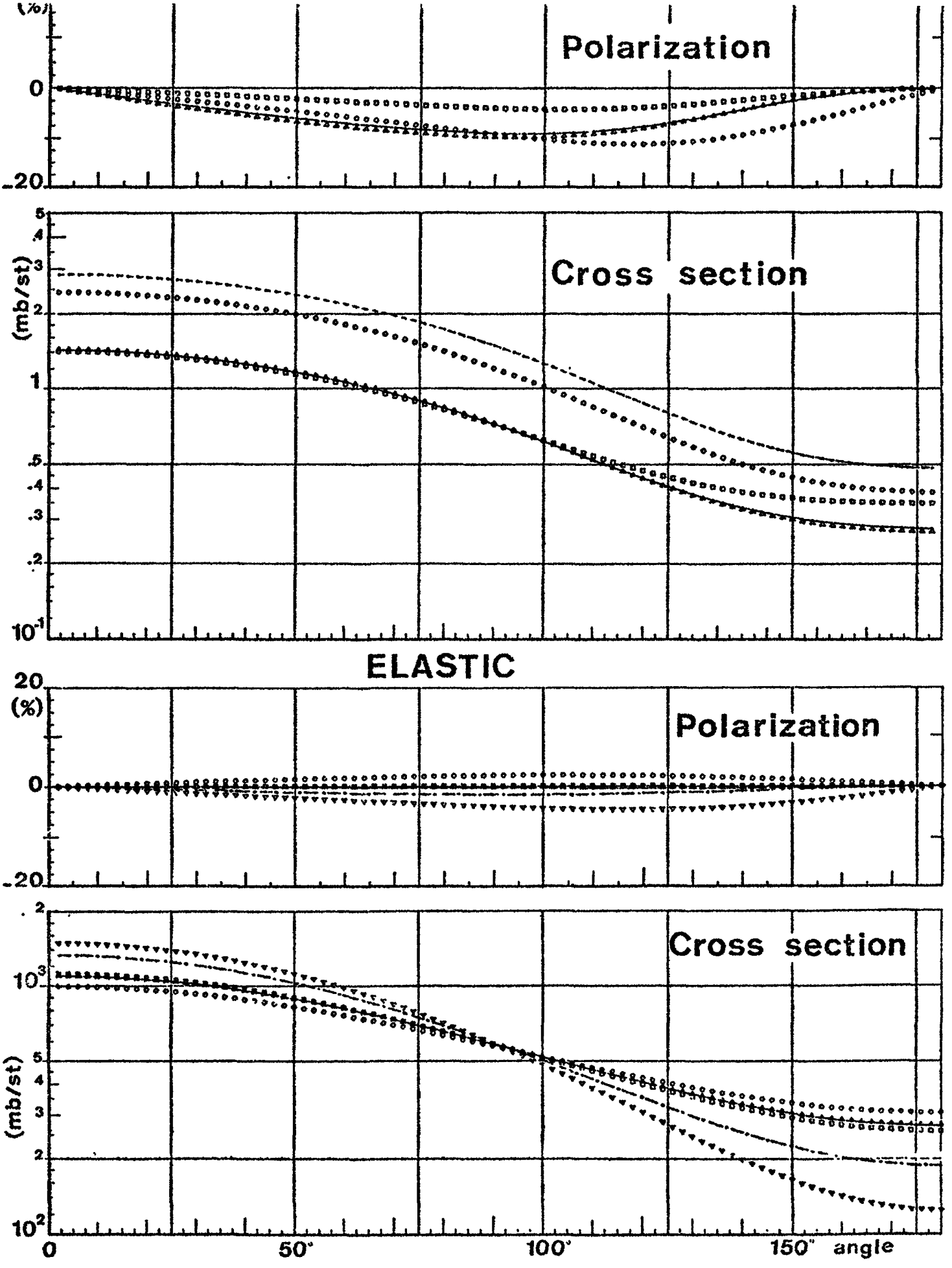

Fig. 6 Effect of Number of Coupled Levels at 0. 1 MeV

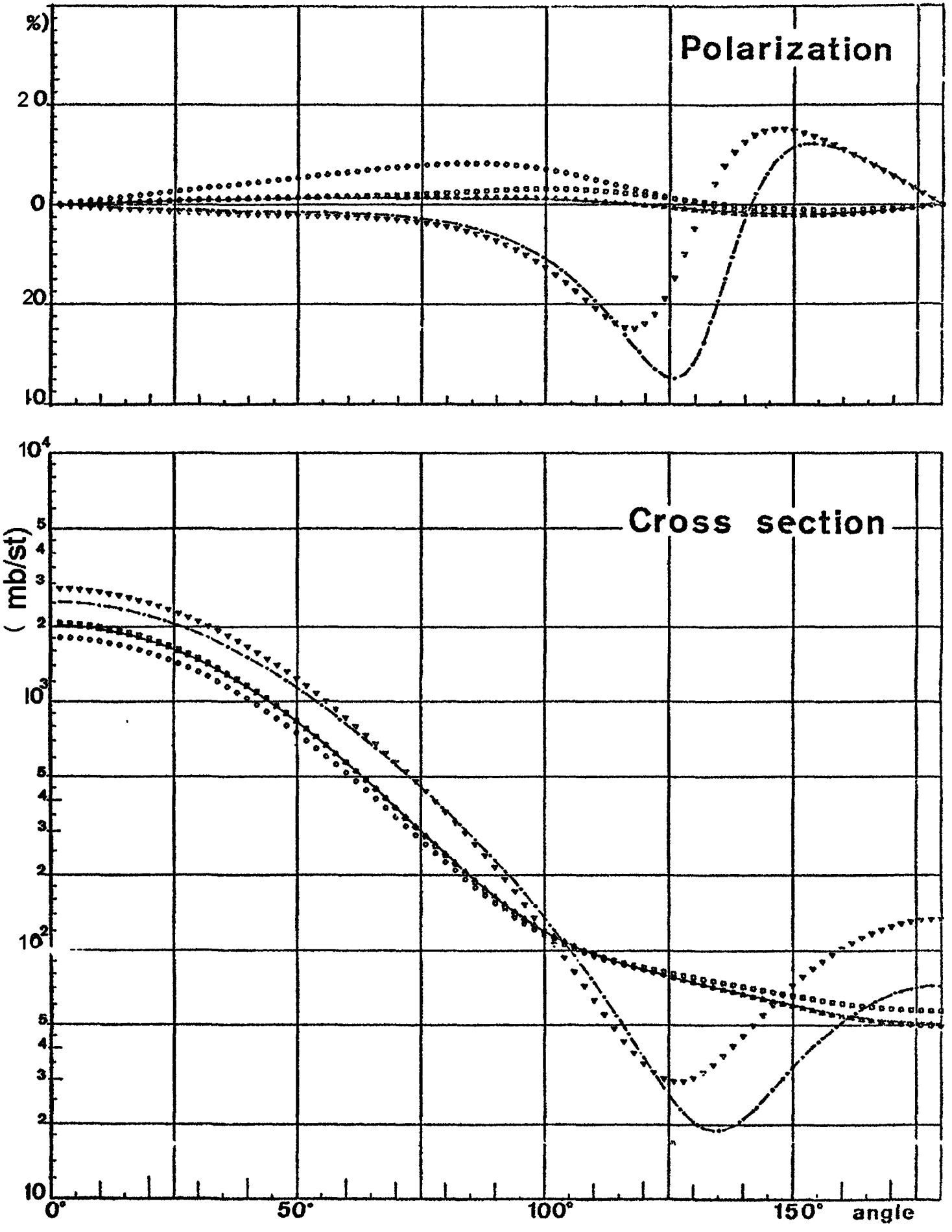

Fig. 7A Effect of Number of Coupled Levels at 0.6 MeV (elastic scattering)

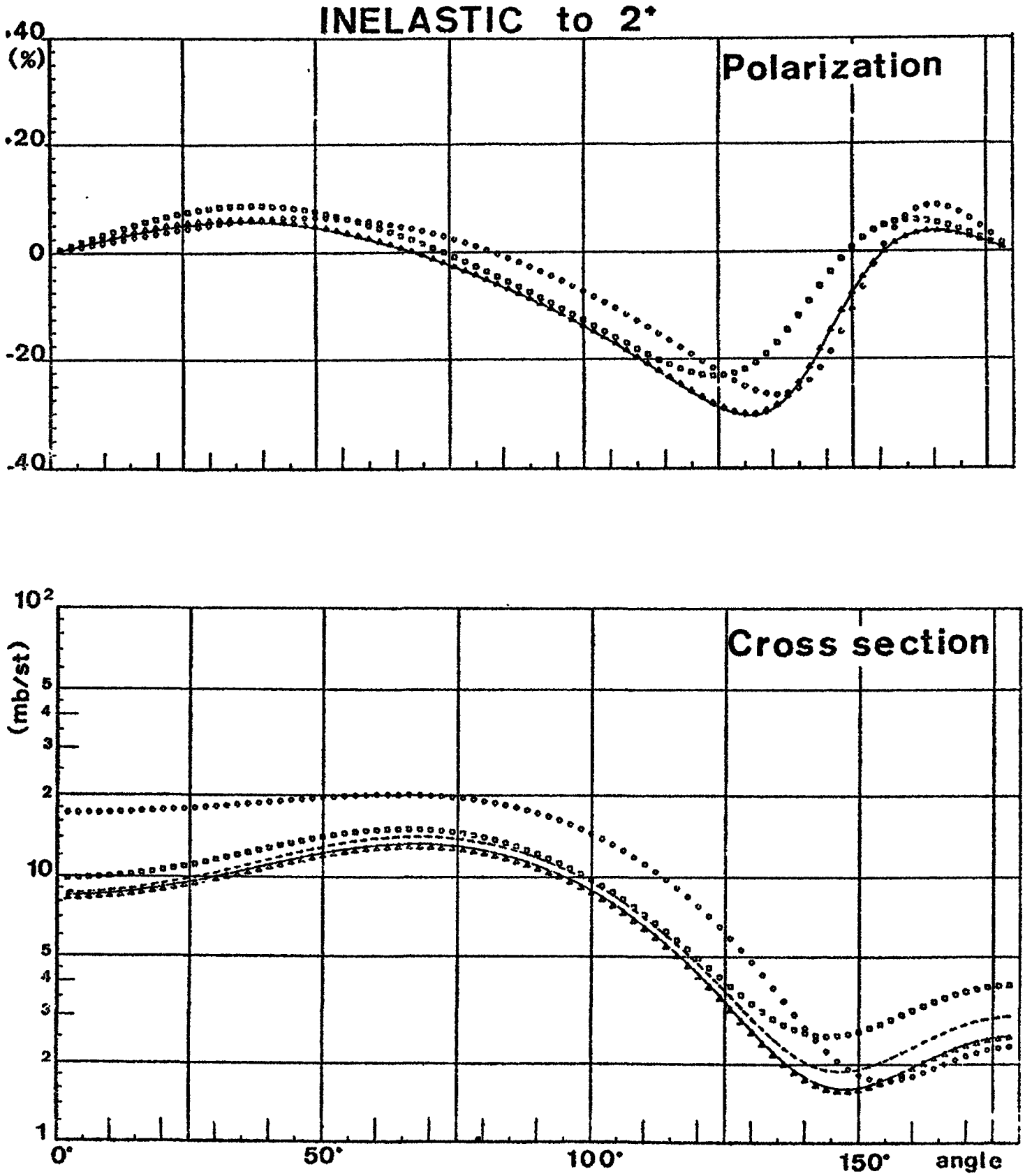

Fig. 7 B Effect of Number of Coupled Levels at 0.6 MeV
(inelastic scattering to the 2^+ state)

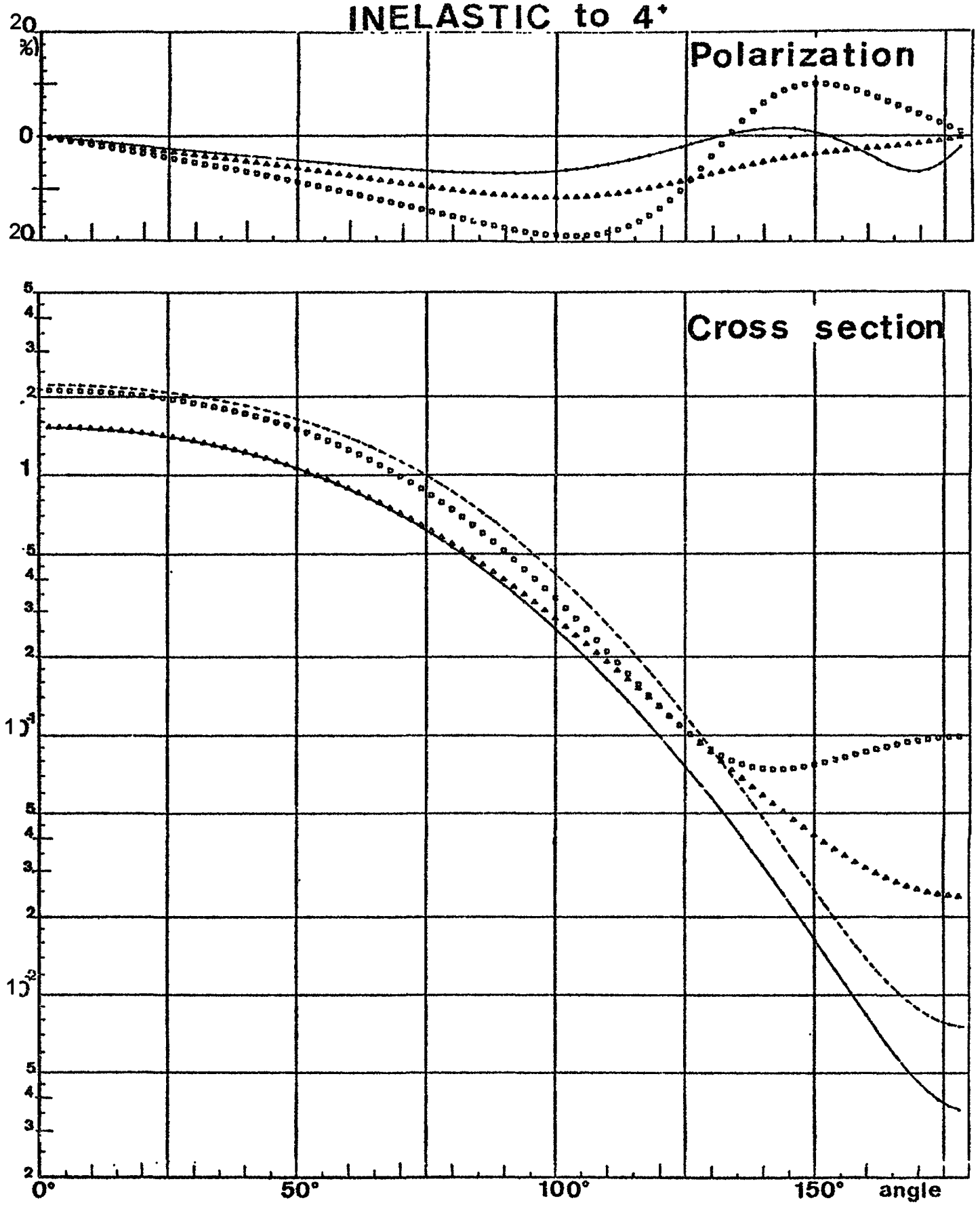

Fig. 7 C Effect of Number of Coupled Levels at 0.6 MeV
(inelastic scattering to the 4^+ state)

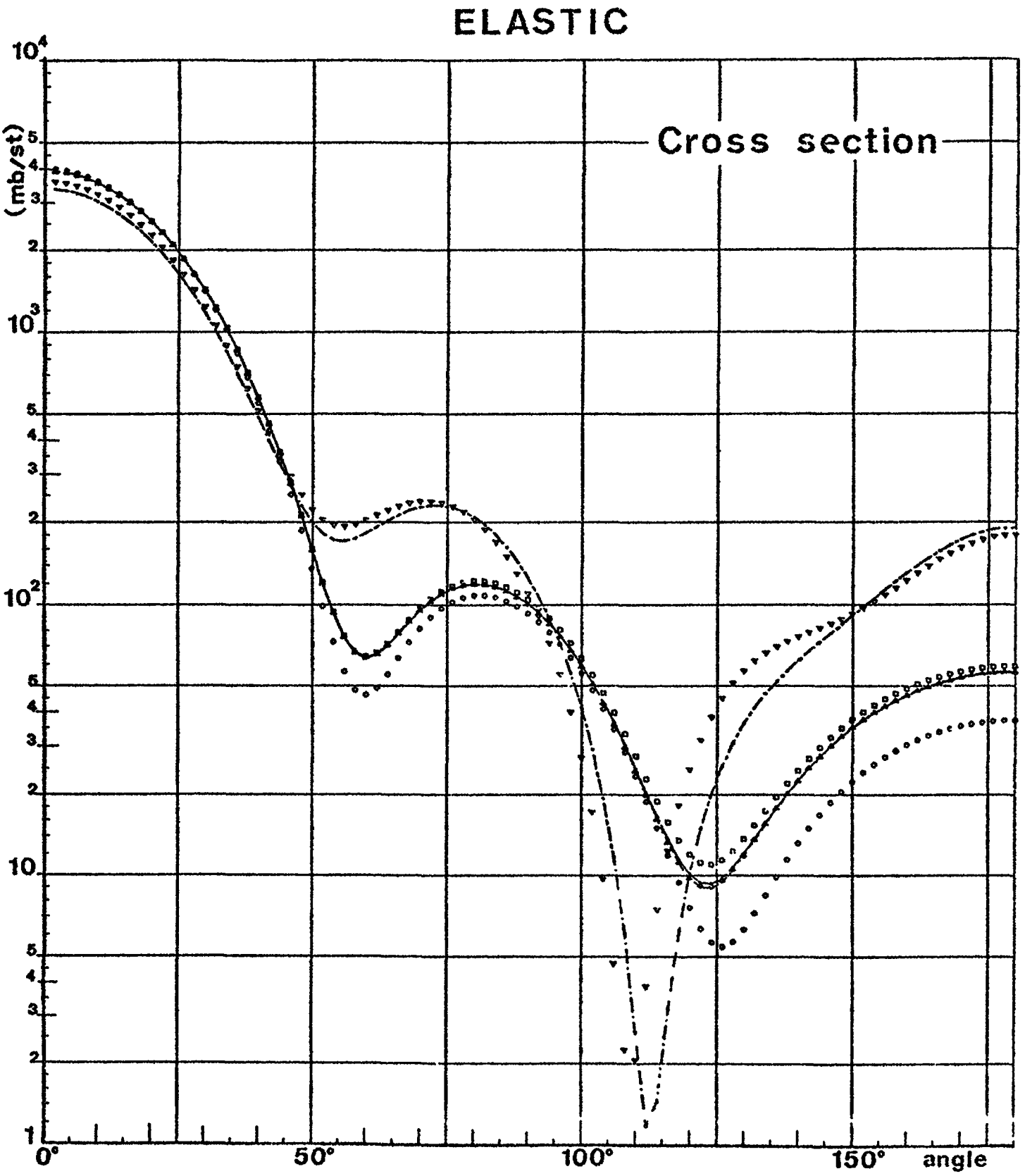

Fig. 8 A Effect of Number of Coupled Levels at 2 MeV
(elastic scattering cross section)

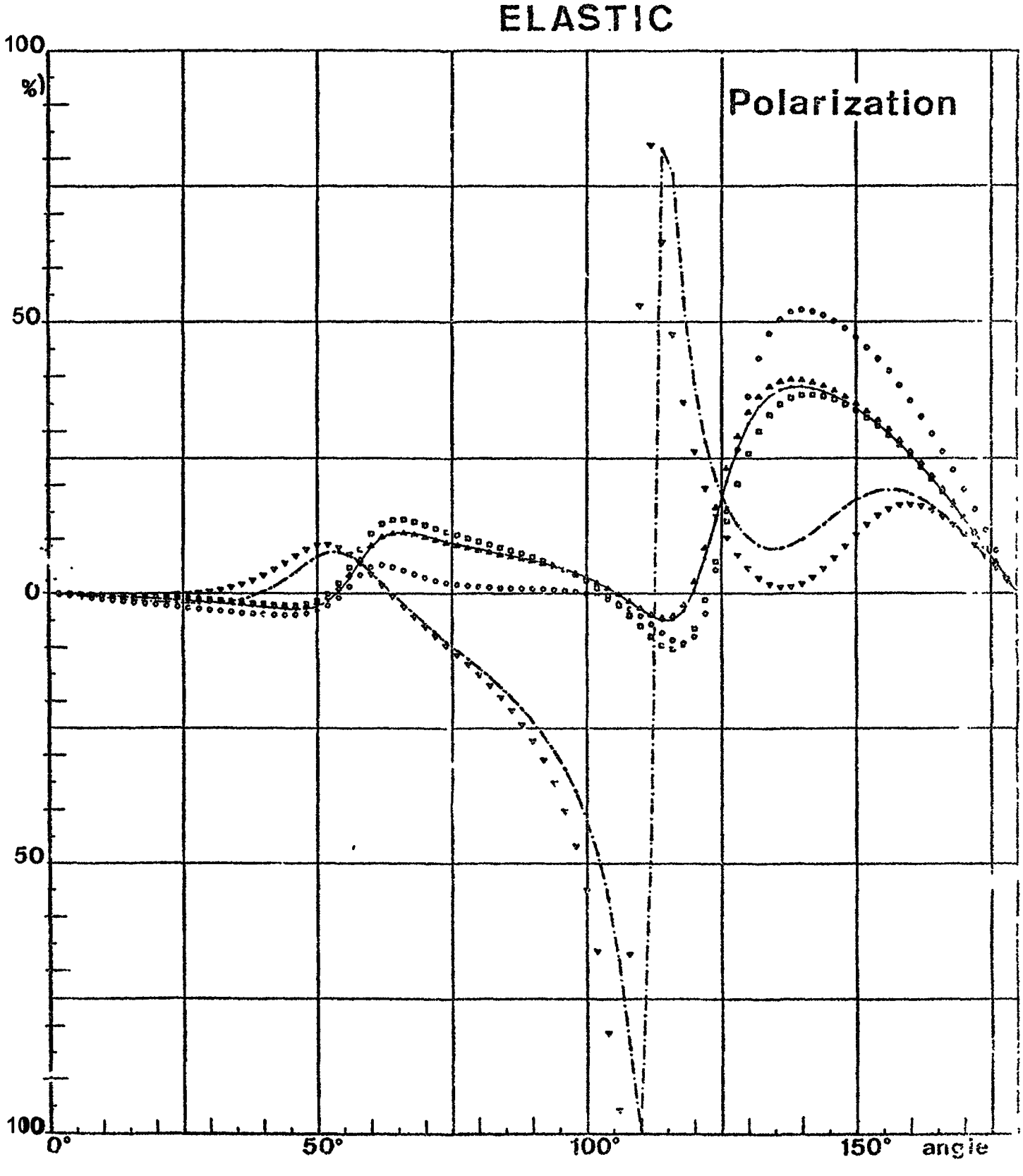

Fig. 8 B Effect of Number of Coupled Levels at 2 MeV
(polarization of elastic scattering)

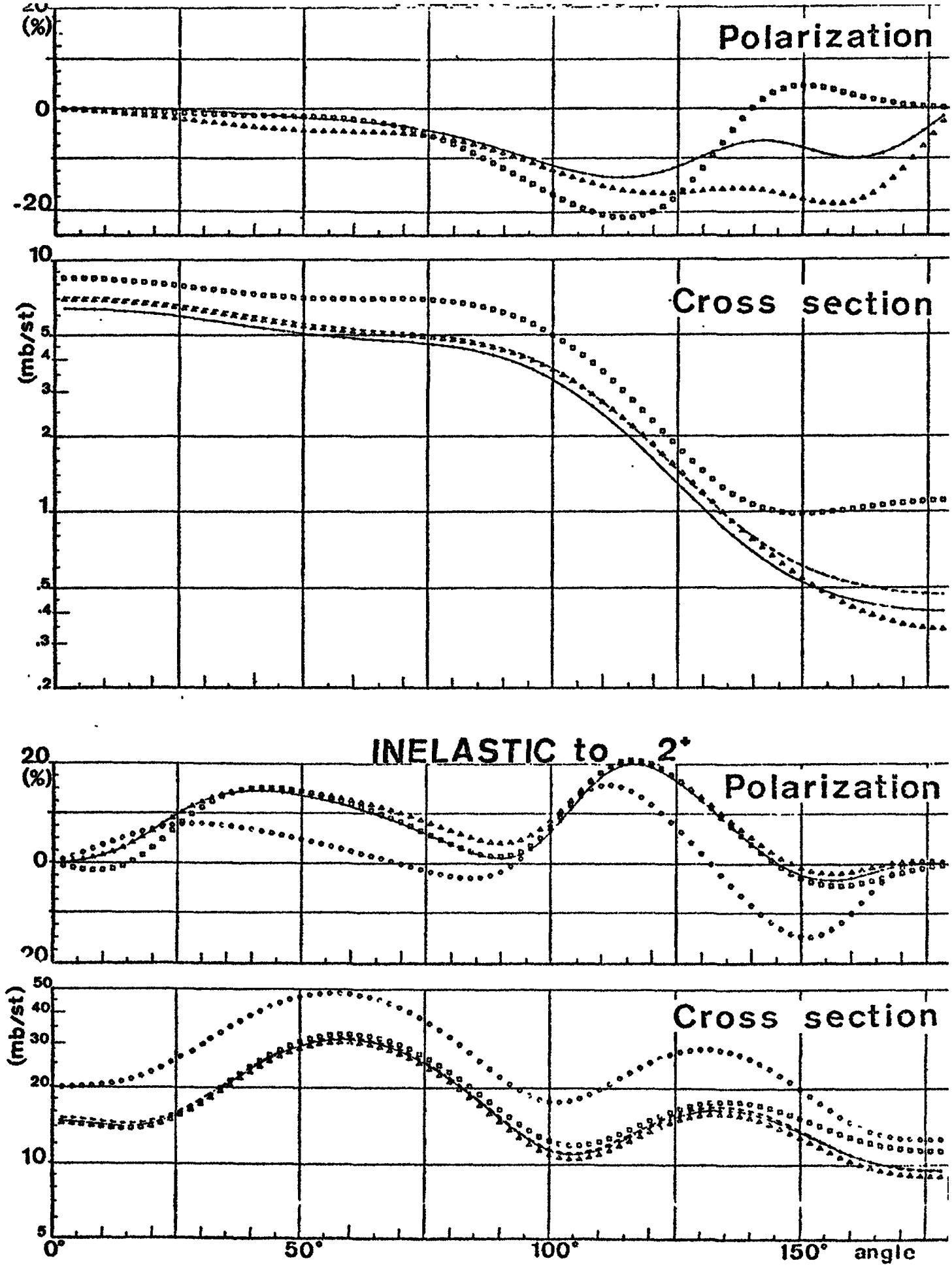

Fig. 8 C Effect of Number of Coupled Levels at 2 MeV (inelastic scatterings)

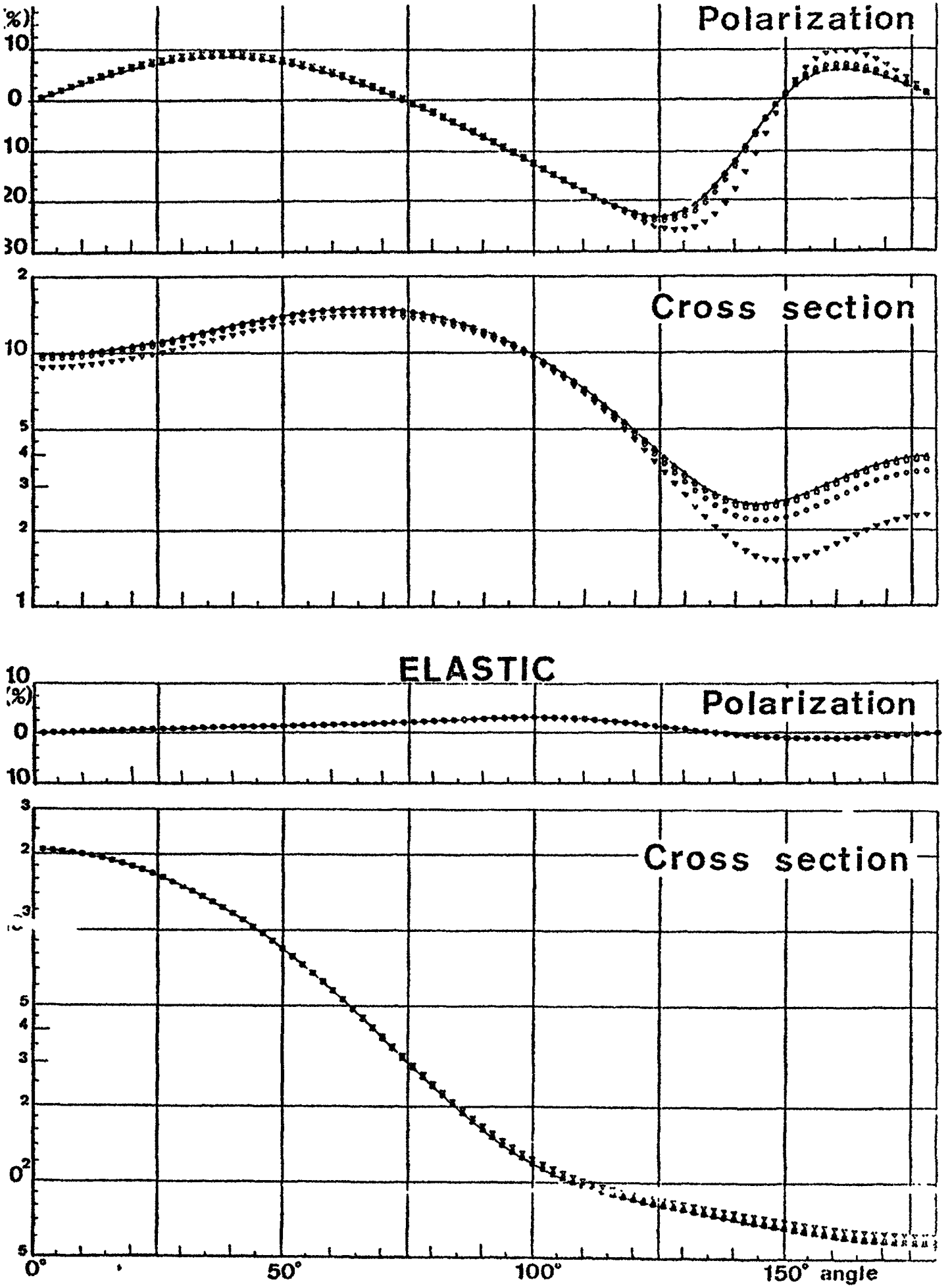

Fig. 9 Effect of mesh interval at 0.6 MeV

(— : 0.1 fm, Δ : 0.3 fm, □ : 0.5 fm, ○ : 0.75 fm, ▽ : 1.0 fm)

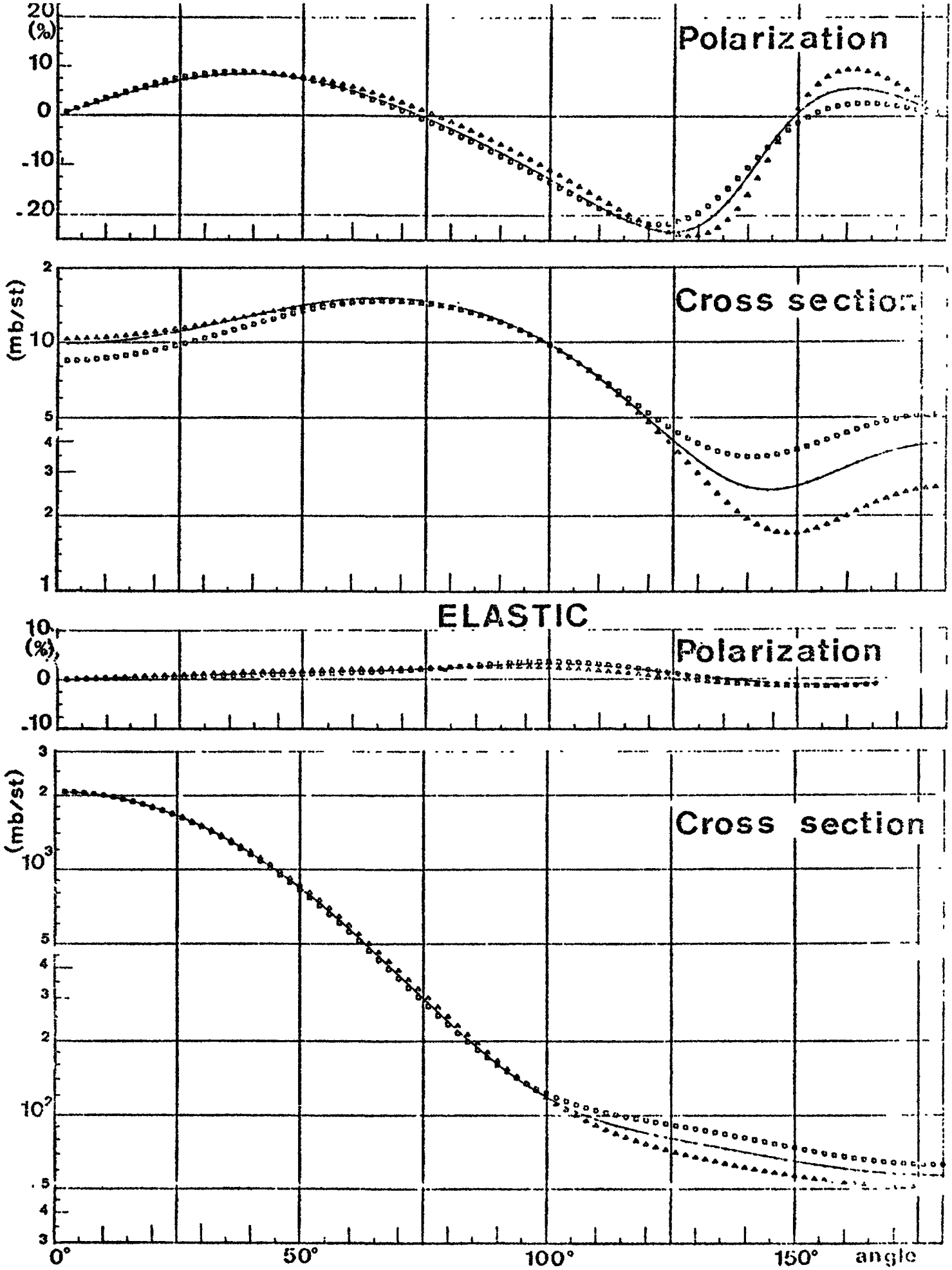

Fig. 10 A Effect of β_2 - value at 0.6 MeV

(— : $\beta_2 = 0.24$, Δ: $\beta_2 = 0.22$, ○ $\beta_2 = 0.26$)

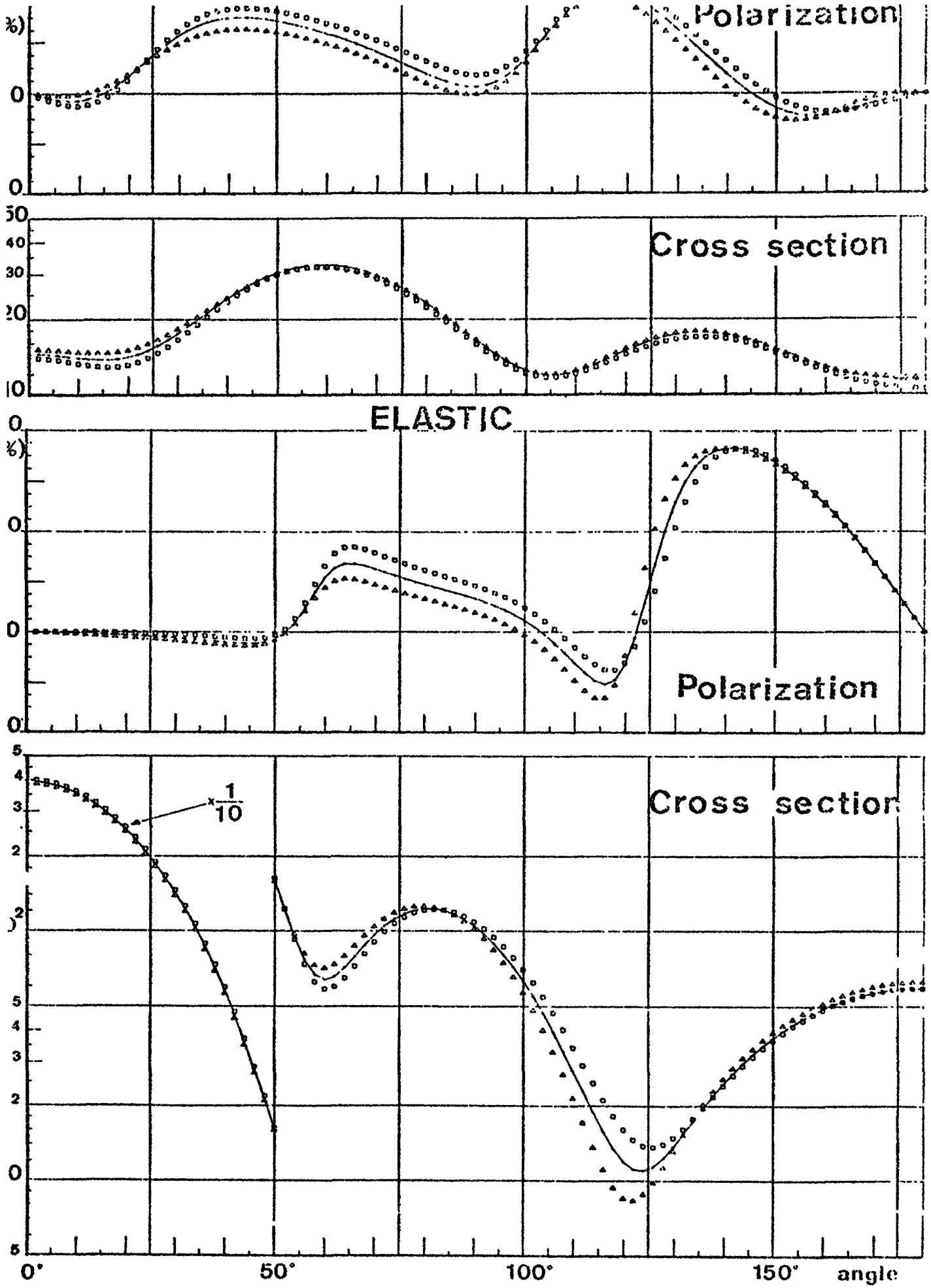

Fig. 10 B Effect of β_2 - value at 2 MeV

(— : $\beta_2 = 0.24$, Δ : $\beta_2 = 0.22$, o $\beta_2 = 0.26$)

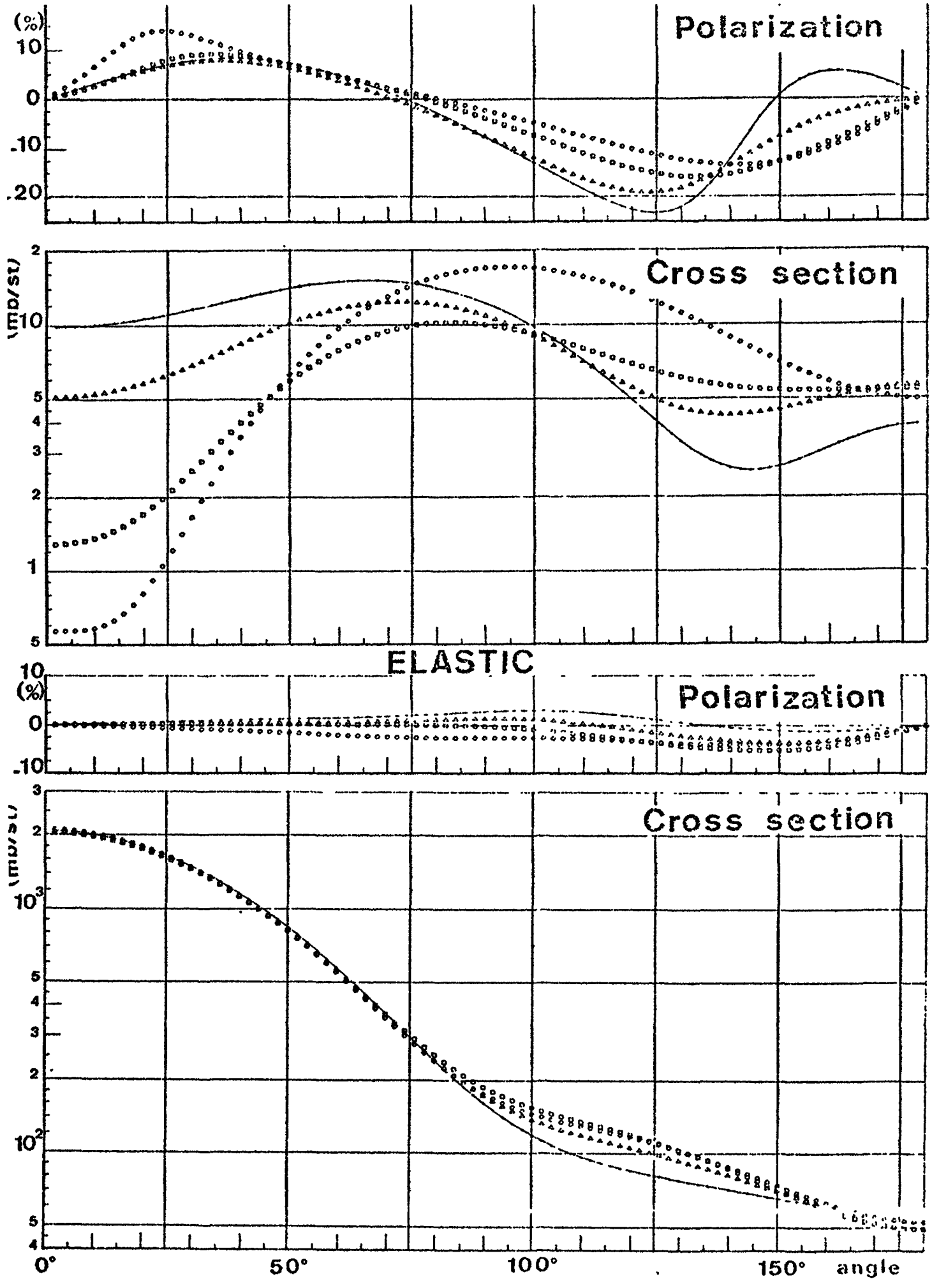

Fig. 11 A Effect of β_4 value at 0.6 MeV ($\beta_2 = 0.24$)

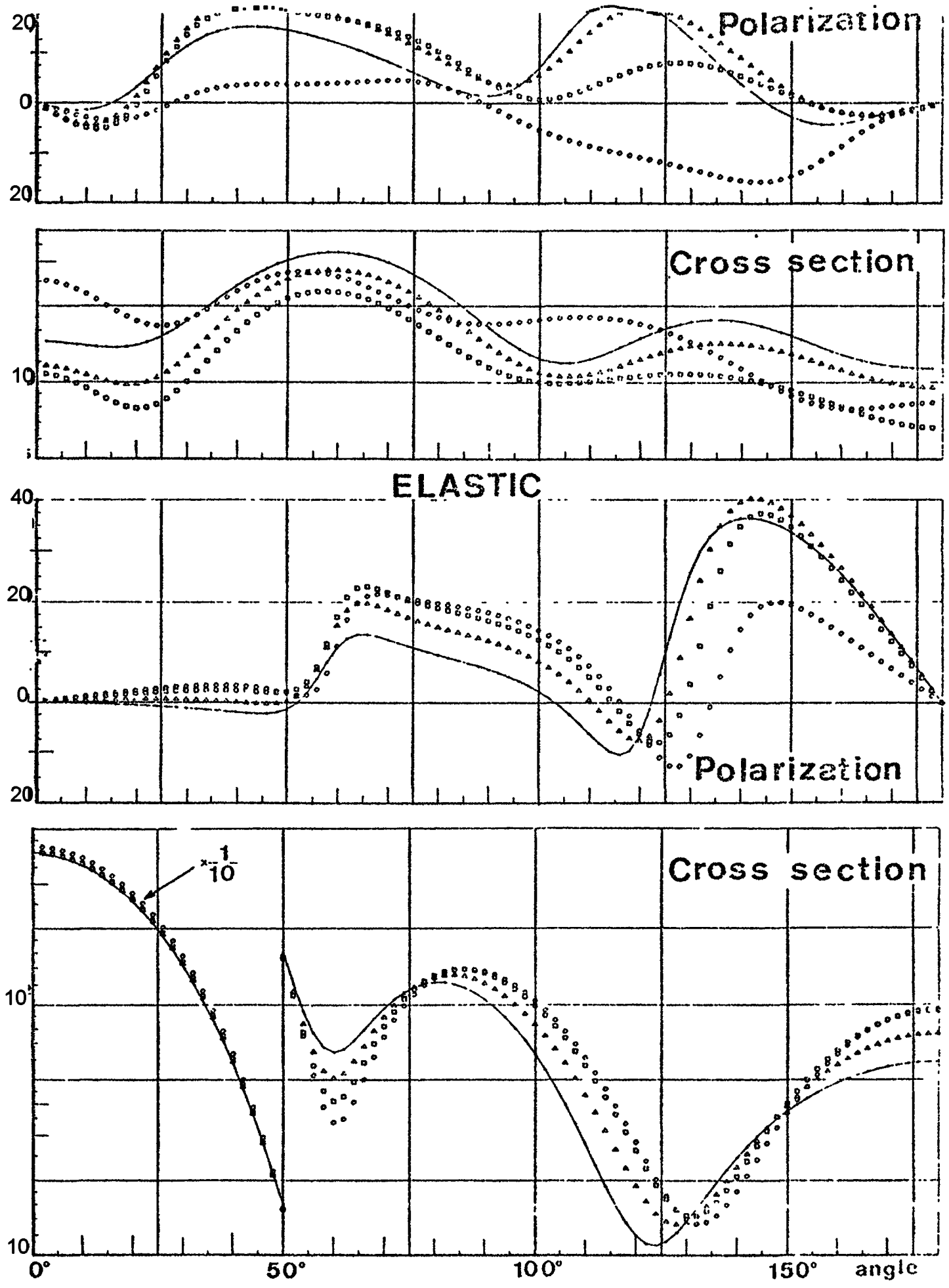

Fig. 11 B Effect of β_4 value at 2 MeV ($\beta_2 = 0.24$)

(— : $\beta_4 = 0$, Δ: $\beta_4 = 0.05$, □: $\beta_4 = 0.1$, o : $\beta_4 = 0.2$)

APPENDIX I

COMPARISON BETWEEN ECIS 70 AND JUPITOR

The results of the JUPITOR code are compared with those of ECIS 70 under various conditions. They are given in tables A1, A2, A3 and A4. They agree very well with each other except in the case of spherical imaginary potential approximation in table A4. This error is not severe, however, because this approximation should be abandoned according to the discussion in section II.1.

The computing time of JUPITOR seems much longer than those of ECIS 70.* This difference is very interesting and we will discuss it here.

Generally in the coupled channel model we must consider the contributions of a high angular momentum which are negligible in the spherical approximation. This can be understood as follows : without coupling the neutron which enters with a high angular momentum (ℓ-value) must go out with the same high angular momentum. The scattering matrix element is small in this case because the centrifugal force reduces it for both the incoming and outgoing channels. In the coupled channel case, however, the neutron can go out with a lower ℓ-value, leaving the rest of the angular momentum in the target nucleus. Hence the effect of the centrifugal force is weaker in this case and the contributions of higher angular momenta cannot be neglected.

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* At 2 MeV we did not calculate the inelastic scattering to the 4^+ state in order to save the computing time. Hence the time at 2 MeV cannot be compared with those at 0.1 and 0.6 MeV.

There is some difference between ECIS 70 and JUPITOR in controlling the maximum value of the angular momentum. In the ECIS 70 code the maximum value of the total angular momentum of the system (J_{max}) is controlled by the input data. All the possible values of the orbital angular momentum (ℓ) are considered in the coupled equations for any J ($\leq J_{max}$). In the JUPITOR code, on the other hand, it is the maximum value of the optical angular momentum of neutrons (ℓ_{max}) which is controlled by the input. The coupling to the states whose ℓ-value is higher than ℓ_{max} is ignored in the coupled equation.

Without coupling one J^{π}-value corresponds to one ℓ-value. Therefore we can put $\ell_{max} = J_{max} + 1/2$. If the coupling with some excited levels is considered, on the other hand, the contributions of high ℓ-values exist in the coupled equations for a low J-value, and contributions of low ℓ-values exist for a high J-value. Hence the relation between ℓ_{max} and J_{max} is not simple.

From our experience at 0.1 MeV, we must increase J_{max} from 2.5 to 4.5 in ECIS 70 with coupling of 3 levels (0^+, 2^+ and 4^+). In JUPITOR we must increase ℓ_{max} from 3 to 8 in order to obtain the same results as ECIS 70. In this case, JUPITOR calculates coupled equations for very high J-values, which are not significant, and needs more computing time.

As a conclusion, we must increase ℓ_{max} more than J_{max} with increasing number of coupling at least for even-even nucleus.

Table A-1

Comparison of JUPITOR with ECIS70 at 0.1 MeV

Coupling			2 levels		3 levels	
l_{max}			9		9	
σ_r	(mb)		4406	(+0.07%)	4977	(+0.28%)
σ_T	(mb)		11961	(+0.05%)	12730	(-0.09%)
ξ_o	($\times 10^{-4}$)		1.544	(<0.05%)	1.620	(+0.43%)
ξ_1	($\times 10^{-4}$)		2.523	(+0.12%)	3.052	(-0.30%)
C_l^j			Error = value with JUPITOR - value with ECIS70			
l	j^π		Real	Imag.	Real	Imag.
0	$1/2^+$		- 0.0001	+ 0.0001	+ 0.0006	- 0.0005
1	$1/2^-$		+ 0.0001	$<10^{-4}$	+ 0.0004	+ 0.0001
	$3/2^-$		+ 0.0001	$<10^{-4}$	+ 0.0004	+ 0.0001
2	$3/2^+$		$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
	$5/2^+$		$<10^{-4}$	- 0.0001	$<10^{-4}$	$<10^{-4}$
Relative dev.	Elastic	$\frac{d\sigma}{d\Omega}$	0.0003		0.0037	
		P	0.0035		0.0048	
	Inelas. (2^+)	$\frac{d\sigma}{d\Omega}$	0.0024		0.0037	
		P	0.0048		0.023	
Time (sec.)			18		87	
Memory (K bytes)			183		183	

Table A-2

Comparison of JUPITOR with ECIS70 at 0.6 MeV

Coupling			2 levels		3 levels		4 levels	
l_{max}			9		9		9	
σ_r	(mb)		4149	(+0.02%)	4138	(+0.02%)	4140	(<0.02%)
σ_T	(mb)		8907	(-0.02%)	9423	(-0.02%)	9362	(-0.02%)
ξ_o	($\times 10^{-4}$)		1.256	(<0.05%)	1.244	(<0.05%)	1.212	(<0.05%)
ξ_1	($\times 10^{-4}$)		1.990	(+0.10%)	2.005	(+0.05%)	2.049	(+0.05%)
C_l^j			Error = value with JUPITOR - value with ECIS70					
l	j^π		Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$		- 0.0002	- 0.0001	- 0.0001	- 0.0001	- 0.0001	- 0.0001
1	$1/2^-$		+ 0.0002	- 0.0001	+ 0.0001	- 0.0001	+ 0.0002	- 0.0002
	$3/2^-$		+ 0.0003	- 0.0001	+ 0.0002	- 0.0001	+ 0.0002	- 0.0001
2	$3/2^+$		+ 0.0001	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
	$5/2^+$		+ 0.0001	- 0.0001	$<10^{-4}$	- 0.0001	+ 0.0001	- 0.0001
3	$5/2^-$		$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	0.0001
	$7/2^-$		$<10^{-4}$	$<10^{-4}$	+ 0.0001	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
Relative dev.	Elastic	$\frac{d\sigma}{d\Omega}$	0.0008		0.0007		0.0006	
		P	0.004		0.008		0.047	
	Inelas.	$(2^+)\frac{d\sigma}{d\Omega}$	0.0007		0.0008		0.0008	
		P	0.008		0.004		0.026	
Time (sec.)			17		81		244	
Memory (K bytes)			183		183		183	

Table A-3

Comparison of JUPITOR with ECIS70 at 2 MeV

Coupling		2 levels		3 levels		4 levels	
l_{max}		9		9		9	
σ_r (mb)		4297	(<0.02%)	4020	(-0.17%)	4068	(-0.17%)
σ_T (mb)		7767	(+0.01%)	7640	(-0.08%)	7654	(<0.01%)
ξ_o ($\times 10^{-4}$)		0.890	(<0.01%)	0.841	(+0.01%)	0.853	(<0.01%)
ξ_1 ($\times 10^{-4}$)		1.284	(+0.14%)	1.251	(+0.14%)	1.259	(+0.15%)
C_l^j		Error = value with JUPITOR - value with ECIS70					
l	j^π	Real	Imag.	Real	Imag.	Real	Imag.
0	$1/2^+$	+ 0.0001	+ 0.0001	+ 0.0001	+ 0.0002	+ 0.0001	+ 0.0001
1	$1/2^-$	+ 0.0001	- 0.0001	$<10^{-4}$	- 0.0002	$<10^{-4}$	- 0.0002
	$3/2^-$	$<10^{-4}$	- 0.0002	$<10^{-4}$	- 0.0001	- 0.0001	+ 0.0002
2	$3/2^+$	+ 0.0001	- 0.0001	$<10^{-4}$	- 0.0001	+ 0.0002	- 0.0049
	$5/2^+$	$<10^{-4}$	- 0.0001	+ 0.0001	- 0.0001	- 0.0040	- 0.0041
3	$5/2^-$	+ 0.0001	+ 0.0001	+ 0.0001	$<10^{-4}$	- 0.0014	- 0.0005
	$7/2^-$	- 0.0001	$<10^{-4}$	+ 0.0001	$<10^{-4}$	- 0.0006	- 0.0004
4	$7/2^+$	+ 0.0001	$<10^{-4}$	+ 0.0010	+ 0.0023	+ 0.0004	+ 0.0026
	$9/2^+$	+ 0.0001	$<10^{-4}$	- 0.0025	- 0.0009	- 0.0018	- 0.0012
Relative dev. Elastic	$\frac{d\sigma}{d\Omega}$	0.0003		0.002		0.002	
	P	0.005		0.083		0.058	
Relative dev. Inelas. (2^+)	$\frac{d\sigma}{d\Omega}$	0.009		0.017		0.035	
	P	0.041		0.182		0.280	
Time (sec.)		15		63		111	
Memory (K bytes)		183		183		183	

Table A-4

Comparison of JUPITOR and ECIS70 at 0.6 MeV

with coupling of 2 levels with special conditions

Condition		Spherical imag. pot. P 4		Deformed imag. pot. P 2	
l_{max}		9		9	
σ_r	(mb)	4221	(+1.1%)	4053	(+0.03%)
σ_T	(mb)	9294	(+1.7%)	8883	(-0.02%)
ξ_o	($\times 10^{-4}$)	1.273	(-0.47%)	1.235	(+0.08%)
ξ_1	($\times 10^{-4}$)	2.019	(+0.65%)	1.929	(+0.05%)
C_l^j		Error = value with JUPITOR - value with ECIS70			
l	j^π	Real	Imag.	Real	Imag.
0	$1/2^+$	+ 0.0087	0.0036	- 0.0001	- 0.0001
1	$1/2^-$	- 0.0030	0.0072	+ 0.0003	- 0.0002
	$3/2^-$	- 0.0036	0.0076	+ 0.0003	$<10^{-4}$
2	$3/2^+$	- 0.0029	0.0016	+ 0.0001	- 0.0001
	$5/2^+$	- 0.0033	0.0015	+ 0.0001	$<10^{-4}$
3	$5/2^-$	- 0.0002	0.0003	+ 0.0001	$<10^{-4}$
	$7/2^-$	- 0.0004	0.0004	$<10^{-4}$	$<10^{-4}$
Relative dev. Elastic	$\frac{d\sigma}{d\Omega}$	0.032		0.001	
	P	0.082		0.004	
Relative dev. Inelas. (2^+)	$\frac{d\sigma}{d\Omega}$	0.068		0.001	
	P	0.053		0.008	
Time (sec.)		15		16	
Memory (K bytes)		183		183	

APPENDIX II

The ADAPE-code was originally written at Bologne for an IBM 7094. This program uses two scratch tapes in order to save the size of memory.

One of these scratch tapes records all the C-matrix coefficients after solving the coupled equations and are reread at the stage of calculating the cross sections.

In the actual calculation this scratch tapes is reread so often (theoretical maximum : 40,000 times) that not only the I/O time but also the CP running time increases very much.

Running this program on an IBM 360/91 computer at Saclay, we tried to avoid this scratch tape by keeping all the C-matrix coefficients in the core memory. The improvement of computing time is very important though we must increase the size of core memory from 130 K bytes to 190 K bytes. For example, with neutrons whose energy is 14 MeV and with $l_{max} = 15$ the CP running time is improved from 900 sec to 200 sec and the I/O time from 7600 sec to 30 sec.

COMPARISON OF SPHERICAL OPTICAL MODEL CODES AND STANDARD VALUES FOR NUCLEAR DATA EVALUATIONS

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ABSTRACT

In order to examine the reliability of the results calculated with different spherical optical model codes and to find the best conditions of numerical integration, six codes (MAGALI, GENOA, KOUAC, ABACUS-2, JUPITOR and ECIS 70) were compared with the same optical model parameters for neutrons whose energies are 0.6, 1.75 and 14.1 MeV.

The number of meshes in the numerical integration should be determined to optimize both truncation error and round-off error. The best value should fall between 100 and 200 for a code with single precision in IBM-360. An insufficient matching radius causes considerable errors (as in the case of GENOA). On the other hand, a slight difference of the physical constants used in the programme, such as the neutron mass and the conversion constant between energy and wave length, causes a fairly big error on the results (as in the case of ABACUS-2). Taking these conditions into consideration, we found that the results of these six codes agree very well with each other.

It seems very dangerous to use some code as a black box without careful examination about these conditions. Hence we propose these present results as some standard values to check other codes.

I INTRODUCTION

We have a project to evaluate the strength function, the angular distribution and the inelastic scattering cross section systematically for various nuclei whose experimental data are not sufficient for the reactor calculation. The optical model is a very useful tool for this project.

There are mamy optical model codes and the results of one code do not always agree with those of other codes. It was recently pointed out that the results of the same program were considerably different for IBM-360 and for CDC-6600. Hence we must know at first the reliability of various optical model programs, the limit of errors, and the best conditions of numerical calculation.

Most of the nuclei are not spherical and the coupled channel calculation is required. In this note, however, we shall discuss the spherical case only. The same type of examination is now under work for the coupled channel codes.

II COMPARISON OF THE PRESENT CODES.

The optical model codes that we use are shown in table 1. These codes are written by different authors and can be considered independent, except MACALI and ECIS70, which were written by Raynal with the same numerical integration method. Though ECIS70 and JUPITOR are the coupled channel codes, we use them as spherical codes without any coupling.

With these 6 codes, C-matrix coefficients, s- and p-wave strength functions, differential elastic cross sections, polarizations, total reaction cross sections and total elastic cross sections were calculated for ^{40}Ca and ^{238}U at 0.6, 4.75 and 14.1 MeV. The optical potential used in this test in shown in Table 2.

In order to check the round-off error, whose significance will be discussed in section III, 54 bits CDC-6600 was also used for the programs with single precision. The conditions of numerical integration are according to the recommended values in the manual (for GENOA and JUPITOR) or to the values usually used at Saclay (for MAGALI and ECIS70). These conditions are tabulated in Table 3.

As all the cases have the same tendency, we will discuss here the results of ^{238}U at 4.75 MeV. The results are tabulated in Table 4. On this table we take the results of MAGALI as standard values, because they are found the most reliable from the following discussions on the mesh interval and the precision.

A) C-matrix coefficients :

The values of C-matrix coefficients are given for MAGALI and the differences from the values of MAGALI are given for the other codes.

The differences of GENOA-IBM, GENOA-CDC, KOUAC-CDC, JUPITOR-IBM, JUPITOR-CDC and ECIS70 are less than 10^{-3}. The differences of KOUAC-CDC seem the smallest of these six and those of GENOA-IBM the largest. The differences of KOUAC-IBM is of the order of 10^{-3} and larger than the preceding six. The results of ABACUS are very different from the others and the errors are of the order of 10^{-2} but seem very random with J^{π} value.

B) Total cross sections :

Only the results of ABACUS deviate by 1% from those of the others. The deviation of ABACUS seems surprisingly small, considering the large deviation in the C-matrix coefficients. The random signs of the deviation in the C-matrix must cancel each other.

C) Strength function :

S-wave and p-wave strength functions are calculated from the C-matrix coefficients. The results of ABACUS deviate from the others by 3 to 4% ; among the others the error of KOUAC-IBM is the largest. Considering the large experimental errors of the strength function, we can say that the results of all the codes except ABACUS agree very well.

D) Differential elastic cross sections and polarization :

The differential elastic cross section and the polarization are calculated from 2° to 180° with 2° intervals, and the χ^2-value from the results of MAGALI are given. From these values, we can conclude the following tendency very easily :

1) The results of ABACUS deviate very much.

2) The results with CDC-6600 deviate less than those with IBM-360.

3) This difference (between CDC 6600 and IBM 360) is very large for KOUAC and ABACUS whose mesh interval is small, and small for GENOA and JUPITOR whose mesh interval is large. This tendency can be interpreted as due to the round-off error and will be discussed in next section.

4) The deviation of GENOA is larger than those of KOUAC-CDC and JUPITOR. This can be interpreted as due to the small matching radius and will be discussed in next section.

E) Time consideration :

Computer times are given in the table. These values are those necessary to calculate the three energies (0.6, 4.75 and 14.7 MeV) at the same time. Computer time depends strongly on the mesh interval. Hence it is difficult to compare these given values.

III ERROR DISCUSSIONS.

Before discussing the results of this comparison, we will discuss the main origins of errors, i.e., the truncation error, the round-off error and the error due to the finite matching radius.

A) Truncation error and round-off error :

These two errors depend on the mesh interval. If we take a smaller mesh interval, the truncation error decreases but the round-off error increases and vice versa. We examined these errors by changing the mesh interval in KOUAC-code.

Fixing the matching radius as 16 fm, we chose the mesh of 400, 200, 100 and 50 steps, i.e., the mesh intervals of 0.04, 0.08, 0.16 and 0.32 fm respectively, and calculated with both CDC-6600 and IbM 360. We take the results with the smallest mesh interval (0.04 fm) in CDC-6600 as the standard values, as the round-off error can be neglected in CDC-6600.

The differences of some C-matrix coefficients are shown in Figs. 1A and 1B. The increasing error in CDC-6600 with decreasing steps can be interpreted as due to the truncation error. This error is negligible with more than 100 steps but becomes large with 50 steps. On the other hand, in IBM-360, the error is the largest with 400 steps, is smallest when the number of steps between 200 and 100 and increases again with 50 steps. The large error with 400 steps is interpreted as the round-off error in this case. The error with 50 steps agrees well with the error in CDC-6600. This suggest that the round-off error becomes very small with 50 steps.

The same tendency is obtained in the χ^2- values of the differential cross section and of the polarization. They are shown in Fig. 2.

From these results, we can conclude :

1) In order to keep the precision of the C-matrix coefficients of the order of 10^{-3}, the mesh step should be between 100 and 200 for the code with the single precision in IBM-360.

2) For the code with the double precision or for the code in CDC-6600, we can keep the precision of the order of 10^{-4} by using a mesh of more than 200 steps.

3) The recommended mesh interval (0.1 fm) for JUPITOR and GENOA is proved to be reasonable.

4) The mesh interval of 0.04 fm (400 steps) for KOUAC and ABACUS is too small for IBM-360 and results in the large round-off error.

B) <u>The error due to the finite matching radius</u> :

The C-matrix should be calculated theoretically at $r = \infty$ but is actually calculated at the point beyond which the effect of the nuclear potential is negligible. The matching radius is :

(1) given as input in ECIS-70 and ABACUS

(2) calculated from the potential strength in MACALI, KOUAC and JUPITOR

(3) calculated from the geometrical parameters in GENOA.

In order to examine this error, the C-matrix coefficients are calculated at various distances and are compared with the values at r = 17 fm. The absolute values of the error are shown in Fig. 3. We used KOUAC with CDC-6600.

For small ℓ-value, the error is small enough (10^{-5}) beyond 14 fm. For large ℓ-value, the error is still of the order of 10^{-4} at r = 15 fm. Considering their $(2\ell + 1)$ weight in the contribution to the cross section, an error of 10^{-4} for $\ell = 6$ corresponds to an error of 10^{-3} for $\ell = 0$.

From this examination, the matching radius for ^{238}U should be more than 15 fm. The matching radius of GENOA (13.6 fm) may be too small.

IV PHYSICAL CONSTANTS.

Among 6 codes, only ABACUS gives different results from those of the other codes. As we put the same conditions of numerical integration as KOUAC, this error is not due to the three origins discussed in section III.

Benzi and Fabbri[7] pointed out that ABACUS code has a different conversion constant between energy and wave number and that this made a considerable difference in the results. We will discuss this point in this section.

The wave number k is defined as :

$$k = \frac{1}{\lambda\!\!\!^{-}} = \frac{\sqrt{2\mu E_{CM}}}{\hbar}$$

where μ is the reduced mass and E_{CM} is the energy in the center of mass system. If we use the units of $(fm)^{-1}$ for k, the atomic mass unit for μ and MeV for E_{CM}, k is expressed as ;

$$k = 0.2187315 \sqrt{\mu E_{CM}} \quad ,$$

with[8] 1 eV = $1.6021917 \times 10^{-12}$ erg

$\hbar = 1.0545919 \times 10^{-27}$ erg. sec

1.a.m.u. = 1.660531×10^{-24} g (C^{12} standard).

This relation can be rewritten as ;

$$k = 0.2187315 \sqrt{m} \left(\frac{M}{M + m}\right) \sqrt{E_{lab}} \quad , \qquad (A)$$

where m is the mass of the incident particle, M the mass of the target nucleus and E_{lab} the energy in the laboratory system. Putting m = 1.0086652 for the neutron mass, we obtain the relation for neutron :

$$k = 0.219677 \left(\frac{M}{M + m}\right) \sqrt{E_{lab}} \qquad (B)$$

These two expressions (A) and (B) give the same results, if the correct m_n-value (1.0086652) is used. However when the approximation of $m_n = 1.0$ is used, the expression (B) gives a much more precise k-value than (A), because the error due to $\sqrt{m}$ is 0.43% and the error due to $\left(\frac{M}{M + m}\right)$ is, on the other hand, 0.04% for M = 20 and 0.004% for M = 200.

The type of expression and the conversion constant used in the present six codes are tabulated in Table 5. Only ABACUS code has type - B expression and all the others have type -A. The conversion constant are nearly 0.2187 for all but ABACUS and are a little lower than the value in equation (A). The constant of ABACUS is based on the old neutron mass data (m = 1.008982) and higher than the value in equation (B).

From this discussion, we get a very ironical conclusion :

1) The results of all the other codes are not correct in spite of their good agreement because the inappropriate combination of type-A expression and $m_n = 1.0$ approximation is used.

2) The results of ABACUS are not correct, because it has old physical constants.

In order to examine this problem, we compare the results calculated with KOUAC with the following four conditions.

N°	conversion constant	m_n	Type
1	0.2178 (original)	1.	A
2	0.2178315	1.	A
3	"	1.0086652	A
4	0.2196770	1.	B

The results are given in Table 6, from which we conclude :

1) With a change of 0.015% of the conversion constant between (1) and (2), the maximum change of C-matrix coefficient is 1% and the changes in strength functions are about 0.1%.

2) With type-A expression, the use of approximation $m_n = 1$ (0.87%) induces changes of the C-matrix-coefficients which are less than 10% and changes of the strength functions whose values are about 2.5% (from (2) and (3)).

3) With type -B expression, on the other hand, the use of approximation $m_n = 1$ makes little error (from (3) and (4)).

We modified the conversion constants in ABACUS and calculated with the same conditions as (3). The results are also given in Table 6. Agreement is now sufficient.

Hence we can conclude now that the disagreements between ABACUS and the other codes are due to adoption of different conversion constants between k and E.

V CONCLUSION.

The results of all the codes except ABACUS agree well with each other, if we choose the appropriate condition for the numerical integration.

The results of the code with the double precision or of the code for CDC-6600 are better than those with the single precision for IBM-360. However the results with the single precision for IBM-360 can sufficiently precise (of the order of 10^{-3} in the C-matrix coefficients) for the actual calculation, if the mesh steps are taken between 100 and 200.

The results of GENOA are a little bit deviated from the others. This may be due to its small matching radius. GENOA code is, however, unpublished and we are not allowed to modify it.

The results of ABACUS seem to be deviated from those of the others. But it is found that this deviation is caused by the different values of the physical constants, and that the results agree well with those of the others with the same constant.

The physical constants such as neutron mass and the conversion constant between energy and wave number should be checked carefully. Different values of physical constants change the results considerably. If type-A expression is used in the program, the approximation of $m_n = 1$ makes the maximum error of $\sim$ 10% in C-matrix coefficient and an error of $\sim$ 2.5% in strength function.

VI STANDARD VALUES FOR TESTING A CODE.

MACALI, GENOA, KOUAC, ABACUS and JUPITOR are made by different authors and can be considered to be independent of

each other. The results of these independent codes agree well with each other, if we use the appropriate conditions for numerical integration and the same physical constants. Hence we can rely on these results.

On the other hand, however, it is also found that even a good code can give false results with inadequate usage. Hence it is very dangerous to use a existing code as a black box without careful examination.

We tabulated here the results for ^{40}Ca (light nuclide) and ^{238}U (heavy nuclide) at low (0.6 MeV), medium (4.75 MeV) and high (14.1 MeV) energies. They are calculated wich CDC-6600 by KOUAC with the optical model parameters given in Table 2 with the ideal conditions, i.e. 200 steps of numerical integration, $m_n = 1.0086652$ a.m.u. and $k = 0.2187315\sqrt{\mu E}$.

The limits of error are estimated from comparison of the results of MAGALI, KOUAC-CDC, JUPITOR-CDC and ECIS-70, whose conditions of numerical integrations were found sufficiently adequate.

We propose these values as the standard values and it is recommended to check a program with the same conditions of these values before using it as a black box.

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The preparation of the tables and figures by Mrs Laurent-Guy and Miss Larivet is much appreciated.

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TABLE 1 SPECIFICATION OF CODES COMPARED IN THIS NOTE

NAME	CHANNEL COUPLING	PRECISION	AUTOMATIC SEARCH
MAGALI[1]	single	double	at each energy point
GENOA[2]	"	single	at many energy points
KOUAC[3]	"	single	no
ABACUS-2[4]	"	single	at each energy point
JUPITOR[5]	coupled	single	no
ECIS 70[6]	"	double	no

TABLE 2 - OPTICAL MODEL PARAMETER

$$V(r) = V_r \times \frac{1}{1 + \exp(\frac{r - R}{a_r} r)}$$

$$+ 4a_i W_s \left[- \frac{d}{dr} \frac{1}{1 + \exp(\frac{r - R_i}{a_i})} \right]$$

$$+ (\frac{\hbar}{m_\pi c})^2 \frac{V_{so}}{r} \left[- \frac{d}{dr} \frac{1}{1 + \exp(\frac{r - R_r}{a_r} r)} \right] \vec{\ell} \cdot \vec{\sigma}$$

$$R_r = R_i = r_o A^{1/3}$$

$V_r = 49.3$ MeV ; $W_s = 5.75$ MeV ; $V_s = 5.5$ MeV ;

$r_o = 1.25$ fm ; $a_r = 0.65$ fm ; $a_i = 0.7$ fm.

TABLE 3 CONDITION OF NUMERICAL INTEGRATION

For ^{238}U at 4,75 Mev

	MAGALI	GENOA	ABACUS	KOUAC	JUPITOR	ECIS 70
mesh interval (fm)	0.04	0.1	0.04	0.04	0.1	0.1
matching radius (fm)	15.5	13.6	16	16	15	15

TABLE 4A

The results of various code for ^{238}U at 4.75 MeV

NAME	MACALI (Standard)	GENCA	
MACHINE	IBM 360 (double precision)	IBM 360	CDC 6600
ℓ_{max}	9	9	9
σ_r (mb)	3221	3215 (-1.86%)	3213 (- 0.25%)
σ_{el} (mb)	4141	4139 (-0.05%)	4142 (+ 0.02%)
σ_t (mb)	7362	7354 (-0.11%)	7355 (- 0.10%)
ξ_0 ($\times 10^{-4}$)	0.5181	0.5183 (0.04%)	0.5182 (0.02%)
ξ_1 ($\times 10^{-4}$)	0.5986	0.5982 (-0.07%)	0.5981 (- 0.09%)

ℓ	C_ℓ^j	j^π	VALUE Real	VALUE Imag.	ERROR Real	ERROR Imag.	ERROR Real	ERROR Imag.
0		$\frac{1}{2}^+$	- 0.2214	0.3451	+ 0.0006	- 0.0006	+ 0.0001	$< 10^{-4}$
1		$\frac{1}{2}^-$	- 0.1242	0.3092	+ 0.0008	- 0.0005	- 0.0003	- 0.0002
		$\frac{3}{2}^-$	- 0.1015	0.2694	+ 0.0002	- 0.0003	- 0.0004	- 0.0001
2		$\frac{3}{2}^+$	- 0.1792	0.6940	- 0.0003	- 0.0005	+ 0.0001	- 0.0002
		$\frac{5}{2}^+$	- 0.1968	0.6267	- 0.0002	- 0.0006	$< 10^{-4}$	- 0.0001
3		$\frac{5}{2}^-$	- 0.1937	0.7002	- 0.0006	$< 10^{-4}$	- 0.0002	+ 0.0005
		$\frac{7}{2}^-$	- 0.2740	0.6781	- 0.0004	- 0.0001	- 0.0001	+ 0.0006
4		$\frac{7}{2}^+$	0.0000	0.2250	+ 0.0005	+ 0.0004	- 0.0003	- 0.0001
		$\frac{9}{2}^+$	+ 0.0338	0.3494	+ 0.0002	+ 0.0003	- 0.0004	$< 10^{-4}$
5		$\frac{9}{2}^-$	- 0.0793	0.0700	$< 10^{-4}$	- 0.0005	- 0.0005	- 0.0005
		$\frac{11}{2}^-$	- 0.0433	0.0560	- 0.0001	- 0.0005	- 0.0008	- 0.0005

χ^2 - value $\frac{d\sigma}{d\Omega}$		3.13	1.62
p		0.26	0.21
computer time (sec)	3.80	1.9	4.3
memory	250 K ~~bits~~ bytes	215 K ~~bits~~ bytes	135.4 K words

TABLE 4B
The results of various code for ^{238}U at 4.75 MeV

NAME	MAGALI (Standard)	KOUAC	
MACHINE	IBM 360 (double precision)	IBM 360	CDC 6600
ℓ_{max}	9	10	10
σ_T (mb)	3221	3229 (+ 0.25%)	3222 (+ 0.03%)
σ_{el} (mb)	4141	4136 (- 0.12%)	4140 (- 0.02%)
$\sigma_{t.}$ (mb)	7362	7365 (- 0.04%)	7363 (- 0.01%)
ξ_0 ($\times 10^{-4}$)	0.5181	0.5173 (- 0.16%)	0.5181 (0.00%)
ξ_1 ($\times 10^{-4}$)	0.5986	0.5981 (- 0.10%)	0.5986 (0.00%)
C_ℓ^j	VALUE	ERROR	ERROR
ℓ j^π	Real / Imag	Real / Imag.	Real / Imag.
0 $\frac{1}{2}^-$	- 0.2214 / 0.3451	- 0.0007 / $<10^{-4}$	- 0.0001 / + 0.0001
1 $\frac{1}{2}^-$	- 0.1242 / 0.3092	+ 0.0012 / - 0.0011	$<10^{-4}$ / $<10^{-4}$
1 $\frac{3}{2}^-$	- 0.1015 / 0.2694	+ 0.0014 / - 0.0009	$<10^{-4}$ / + 0.0001
2 $\frac{3}{2}^+$	- 0.1792 / 0.6940	- 0.0003 / + 0.0003	$<10^{-4}$ / $<10^{-4}$
2 $\frac{5}{2}^+$	- 0.1968 / 0.6267	- 0.0006 / - 0.0002	- 0.0001 / $<10^{-4}$
3 $\frac{5}{2}^-$	- 0.1937 / 0.7002	- 0.0010 / - 0.0012	$<10^{-4}$ / $<10^{-4}$
3 $\frac{7}{2}^-$	- 0.2740 / 0.6781	- 0.0007 / - 0.0015	$<10^{-4}$ / $<10^{-4}$
4 $\frac{7}{2}^+$	0.0000 / 0.2250	+ 0.0040 / + 0.0013	$<10^{-4}$ / $<10^{-4}$
4 $\frac{9}{2}^+$	+ 0.0338 / 0.3494	- 0.0018 / + 0.0008	$<10^{-4}$ / + 0.0001
5 $\frac{9}{2}^-$	- 0.0793 / 0.0700	+ 0.0027 / + 0.0001	+ 0.0001 / + 0.0001
5 $\frac{11}{2}^-$	- 0.0433 / 0.0560	+ 0.0021 / + 0.0001	+ 0.0001 / + 0.0001
χ^2 - value $\frac{d\sigma}{d\Omega}$		4.58	0.23
χ^2 - value P		0.77	0.01
computer time (sec)	3.80	7.2	5.6
memory	250 K ~~bits~~ bytes	180 K ~~bits~~ bytes	133.6 K words

TABLE 4C
The results of various code for ^{238}U at 4.75 MeV

NAME	MACALI (Standard)	ABACUS	
MACHINE	IBM 360 (double precision)	IBM 360	CDC 6600
ℓ_{max}	9	13	13
σ_T (mb)	3221	3274 (+ 1.65%)	3257 (+ 1.12%)
σ_{el} (mb)	4141	4015 (- 3.04%)	4058 (- 2.00%)
σ_c (mb)	7362	7288 (- 1.00%)	7315 (- 0.64%)
ξ_0 ($\times 10^{-4}$)	0.5181	0.5364 (+ 3.66%)	0.5356 (+ 3.37%)
ξ_1 ($\times 10^{-4}$)	0.5986	0.5803 (- 3.06%)	0.5812 (- 2.89%)
C^j_ℓ ℓ j^π_+	VALUE Real / Imag.	ERROR Real / Imag.	ERROR Real / Imag.
0 $\frac{1}{2}^-$	- 0.2214 / 0.3451	+ 0.0244 / - 0.0123	+ 0.0216 / - 0.0097
1 $\frac{1}{2}^-$	- 0.1242 / 0.3092	+ 0.0174 / - 0.0247	+ 0.0120 / - 0.0213
1 $\frac{3}{2}^-$	- 0.1015 / 0.2694	+ 0.0221 / - 0.0201	+ 0.0154 / - 0.0173
2 $\frac{3}{2}^+$	- 0.1792 / 0.6940	- 0.0068 / - 0.0289	- 0.0030 / - 0.0232
2 $\frac{5}{2}^+$	- 0.1968 / 0.6267	+ 0.0012 / - 0.0337	+ 0.0033 / - 0.0275
3 $\frac{5}{2}^-$	- 0.1937 / 0.7002	- 0.0250 / - 0.0067	- 0.0187 / - 0.0011
3 $\frac{7}{2}^-$	- 0.2740 / 0.6781	- 0.0175 / - 0.0180	- 0.0123 / - 0.0094
4 $\frac{7}{2}^+$	0.0000 / 0.2250	+ 0.0173 / + 0.0245	+ 0.0067 / + 0.0222
4 $\frac{9}{2}^+$	+ 0.0338 / 0.3494	- 0.0043 / + 0.0191	- 0.0094 / + 0.0330
5 $\frac{9}{2}^-$	- 0.0793 / 0.0700	+ 0.0147 / - 0.0038	+ 0.0038 / - 0.0024
5 $\frac{11}{2}^-$	- 0.0433 / 0.0560	+ 0.0177 / + 0.0020	+ 0.0056 / - 0.0020
χ^2 - value $\begin{cases} \frac{d\sigma}{d\Omega} \\ P \end{cases}$		62.36 8.64	30.80 8.13
computer time (sec)	3.80	10.0	14.1
memory	250 K ~~bits~~ bytes	162 K ~~bits~~ bytes	66.3 K words

TABLE 4D

The results of various code for ^{238}U at 4.75 MeV

NAME	MAGALI (Standard)	JUPITOR	
MACHINE	IBM 360 (double precision)	IBM 360	CDC 6600
ℓ max	9	9	9
σ_T (mb)	3221	3222 (+ 0.03%)	3221 (0.00%)
σ_{el} (mb)	4141	4139 (- 0.05%)	4140 (-0.02%)
σ_t. (mb)	7362	7361 (- 0.01%)	7361 (-0.01%)
ξ_0 ($\times 10^{-4}$)	0.5181	0.5180 (- 0.02%)	0.5181 (0.00%)
ξ_1 ($\times 10^{-4}$)	0.5986	0.5985 (- 0.02%)	0.5985 (-0.02%)

C_ℓ^J		VALUE		ERROR		ERROR	
ℓ	j^π	Real	Imag.	Real	Imag.	Real	Imag
0	$\frac{1}{2}^+$	- 0.2214	0.3451	+ 0.0001	- 0.0001	$< 10^{-4}$	$< 10^{-4}$
1	$\frac{1}{2}^-$	- 0.1242	0.3092	+ 0.0001	- 0.0002	$< 10^{-4}$	- 0.0001
	$\frac{3}{2}^-$	- 0.1015	0.2694	+ 0.0002	- 0.0001	$< 10^{-4}$	$< 10^{-4}$
2	$\frac{3}{2}^+$	- 0.1792	0.6940	- 0.0002	- 0.0003	- 0.0001	- 0.0001
	$\frac{5}{2}^+$	- 0.1968	0.6267	- 0.0002	- 0.0003	- 0.0001	- 0.0002
3	$\frac{5}{2}^-$	- 0.1937	0.7002	- 0.0003	$< 10^{-4}$	- 0.0002	+ 0.0001
	$\frac{7}{2}^-$	- 0.2740	0.6781	- 0.002	- 0.0002	- 0.0001	$< 10^{-4}$
4	$\frac{7}{2}^+$	0.0000	0.2250	+ 0.0003	+ 0.0002	$< 10^{-4}$	+ 0.0001
	$\frac{9}{2}^+$	+ 0.0338	0.3494	- 0.0001	+ 0.0005	- 0.0001	+ 0.0003
5	$\frac{9}{2}^-$	- 0.0793	0.0700	+ 0.0001	+ 0.0001	$< 10^{-4}$	$< 10^{-4}$
	$\frac{11}{2}^-$	- 0.0433	0.0560	+ 0.0001	$< 10^{-4}$	- 0.0001	$< 10^{-4}$

χ^2 - value $\frac{d\sigma}{d\Omega}$		1.50	0.26
P		0.10	0.07
computer time (sec)	3.80	14.0	8.7
memory	250 K ~~bits~~ bytes	183 K ~~bits~~ bytes	103.6 K words

TABLE 4E
The results of various code for ^{238}U at 4.75 MeV.

NAME	MAGALI (Standard)		ECIS. 70	
MACHINE	IBM 360 (double précision)		IBM 360 (double precision)	
ℓ_{max}	9		9	
σ_r (mb)	3221		3221 (0.00%)	
σ_{el} (mb)	4141		4140 (-0.02%)	
σ_t (mb)	7362		7361 (-0.01%)	
ξ_0 ($\times 10^{-4}$)	0.5181		0.5181 (0.00%)	
ξ_1 ($\times 10^{-4}$)	0.5986		0.5985 (-0.02%)	
C_ℓ^J	VALUE		ERROR	
ℓ J^π	Real	Imag.	Real	Imag.
0 $\frac{1}{2}^+$	- 0.2214	0.3451	$<10^{-4}$	$<10^{-4}$
1 $\frac{1}{2}^-$	- 0.1242	0.3092	$<10^{-4}$	- 0.0001
1 $\frac{3}{2}^-$	- 0.1015	0.2694	+ 0.0001	- 0.0001
2 $\frac{3}{2}^+$	- 0.1792	0.6940	- 0.0001	- 0.0001
2 $\frac{5}{2}^+$	- 0.1968	0.6267	+ 0.0001	- 0.0002
3 $\frac{5}{2}^-$	- 0.1937	0.7002	- 0.0002	- 0.0001
3 $\frac{7}{2}^-$	- 0.2740	0.6781	- 0.0001	$<10^{-4}$
4 $\frac{7}{2}^+$	0.0000	0.2250	$<10^{-4}$	+ 0.0001
4 $\frac{9}{2}^+$	+ 0.0338	0.3494	$<10^{-4}$	+ 0.0003
5 $\frac{9}{2}^-$	- 0.0793	0.0700	$<10^{-4}$	$<10^{-4}$
5 $\frac{11}{2}^-$	- 0.0433	0.0560	$<10^{-4}$	+ 0.0001
χ^2 - value $\frac{d\sigma}{d\Omega}$			0.23	
$\frac{d\sigma}{d\Omega}_P$			0.06	
computer time (sec)	3.80		5.4	

TABLE 5 - CONVERSION CONSTANT USED IN EACH PROGRAM

Name	Type	Conversion constant
MAGALI	A	0.2187
GENOA	A	0.2187006
KOUAK	A	0.2187
ABACUS	B	0.2198788
JUPITOR	A	0.2187071
ECIS 70	A	0.2187

TABLE 6 COMPARISON WITH VARIOUS PHYSICAL CONSTANT FOR ^{238}U AT 4.75 KeV

N°		KOUAC-1		KOUAC-2		KOUAC-3		KOUAC-4		ASACUS*	
Type		(A)		(A)		(A)		(B)		(B)	
conversion constant		0.2178		0.2178315		0.2178315		0.2196771		0.2196771	
n_a		1.0		1.0		1.0086652		1.0		1.0086652	
ℓ_{max}		10		10		10		10		12	
σ_Σ (mb)		3222		3223		3251		3251		3248	
$\sigma_{e\ell}$ (mb)		4141		4139		4075		4075		4074	
σ_Σ (mb)		7363		7362		7326		7326		7322	
ξ	$\ell = 0$	0.5180		0.5185		0.5320		0.5321		0.5318	
	$\ell = 1$ ($\times 10^{-4}$)	0.5986		0.5981		0.5840		0.5842		0.5847	
c_ℓ^j	J^π	Real	Imag	Real	Imag	Real	Imag	Real	Imag	Real	Imag
$\ell = 0$	$1/2^+$	-0.2215	0.3452	-0.2209	0.3449	-0.2045	0.3375	-0.2045	0.3375	-0.2039	0.3365
$\ell = 1$	$1/2^-$	-0.1242	0.3092	-0.1239	0.3086	-0.1149	0.2921	-0.1149	0.2920	-0.1143	0.2923
	$3/2^-$	-0.1015	0.2694	-0.1001	0.2690	-0.0895	0.2554	-0.0895	0.2553	-0.0888	0.2556
$\ell = 2$	$3/2^+$	-0.1792	0.6940	-0.1793	0.6934	-0.1817	0.6754	-0.1816	0.6754	-0.1820	0.6763
	$5/2^+$	-0.1969	0.6267	-0.1968	0.6260	-0.1943	0.6048	-0.1943	0.6046	-0.1948	0.6057
$\ell = 3$	$5/2^-$	-0.1938	0.7003	-0.1943	0.7003	-0.2090	0.6996	-0.2090	0.6996	-0.2080	0.6992
	$7/2^-$	-0.2741	0.6781	-0.2744	0.6779	-0.2841	0.6707	-0.2841	0.6707	-0.2837	0.6708
$\ell = 4$	$7/2^+$	-0.0000	0.2250	0.00018	0.2256	0.0056	0.2430	0.0056	0.2431	0.0050	0.2408
	$9/2^+$	0.0338	0.3495	0.0336	0.3504	0.0266	0.3765	0.0265	0.3766	0.0274	0.3734
$\ell = 5$	$9/2^-$	-0.0793	0.0701	-0.0792	0.0700	-0.0763	0.0680	-0.0763	0.0680	-0.0765	0.0682
	$11/2^-$	-0.0433	0.0561	-0.0432	0.0561	-0.0388	0.0596	-0.0387	0.0576	-0.0392	0.0573
$\ell = 6$	$11/2^+$	0.0150	0.0269	0.0150	0.0270	0.0153	0.0297	0.0153	0.0297	0.0153	0.0295
	$13/2^+$	0.00279	0.0561	0.00262	0.0562	-0.00258	0.0581	-0.00261	0.0581	-0.00177	0.0578
$\ell = 7$	$13/2^-$	0.00124	0.00178	0.00125	0.00178	0.00138	0.00190	0.00138	0.00190	0.00139	0.00188
	$15/2^-$	0.0292	0.00236	0.00293	0.00237	0.00318	0.00258	0.00318	0.00259	0.00318	0.00255

*This condition is exactly the same as (3)

TABLE 7A STANDARD VALUES FOR ^{40}Ca

(the limit of error in C-matrix coefficients is ± 0.001)

Energy (MeV)		0.6		4.75		14.1	
ℓ_{max}		3		7		10	
σ_r (mb)		1514 ± 5		1561 ± 5		1306 ± 5	
σ_{el} (mb)		1922 ± 5		1996 ± 5		1029 ± 5	
σ_{tot} (mb)		3436 ± 10		3557 ± 10		2335 ± 10	
$\xi 0$ ($\times 10^{-4}$)		1.486 ± 0.005		0.654 ± 0.005		0.317 ± 0.005	
$\xi 1$ ($\times 10^{-4}$		1.527 ± 0.005		0.543 ± 0.005		0.311 ± 0.005	
C_ℓ^j		Real	Imag	Real	Imag	Real	Imag
ℓ	j^π						
0	$1/2^+$	-0.2428	0.3884	-0.1026	0.6350	0.2253	0.6198
1	$1/2^-$	-0.1785	0.1189	-0.1140	0.7903	0.2880	0.4649
	$3/2^-$	-0.1700	0.0934	-0.1769	0.7735	0.2837	0.5410
2	$3/2^+$	0.0038	0.0084	0.0459	0.3644	0.1666	0.3647
	$5/2^+$	-0.0075	0.0134	0.0093	0.5205	0.2543	0.4838
3	$5/2^-$	0.0001	0.0004	-0.0618	0.0845	-0.1653	0.2848
	$7/2^-$	-0.0000	0.0002	-0.0027	0.0789	0.0181	0.2784
4	$7/2^+$			0.0162	0.0220	-0.1511	0.4325
	$7/2^+$			0.0043	0.0468	-0.1863	0.2416
5	$9/2^-$			0.0014	0.0014	0.0080	0.1206
	$11/2^-$			0.0028	0.0018	0.0548	0.2930
matching radius	kr	2.5		6		9	
	r	15		12.8		11.2	

TABLE 7B STANDARD VALUES FOR ^{238}U

(the limit of error in C-matrix coefficients is ± 0.001)

Energy (MeV)		0.6		4.75		14.1	
ℓ_{max}		5		10		16	
σ_r (mb)		4110 ± 5		3251 ± 5		2858 ± 5	
σ_{el} (mb)		6871 ± 5		4075 ± 5		2987 ± 5	
σ_{tot} (mb)		10981 ± 10		7326 ± 10		5845 ± 5	
$\xi 0$ ($\times 10^{-4}$)		0.756 ± 0.001		0.532 ± 0.001		0.317 ± 0.001	
$\xi 1$ ($\times 10^{-4}$		2.607 ± 0.001		0.584 ± 0.001		0.287 ± 0.001	
C_{ℓ}^{j} ℓ	j^{π}	Real	Imag	Real	Imag	Real	Imag
0	$1/2^+$	-0.1194	0.8794	-0.2045	0.3375	0.2038	0.6486
1	$1/2^-$	-0.1916	0.4368	-0.1149	0.2921	0.2791	0.5866
	$3/2^-$	-0.2297	0.4615	-0.0895	0.2554	0.2642	0.6235
2	$3/2^+$	-0.0617	0.0314	-0.1817	0.6754	0.2402	0.5043
	$5/2^+$	-0.0522	0.0331	-0.1943	0.6047	0.2408	0.5819
3	$5/2^-$	-0.0023	0.0155	-0.2090	0.6996	0.2163	0.3185
	$7/2^-$	-0.0097	0.0148	-0.2841	0.6707	0.2562	0.4053
4	$7/2^+$	0.0000	0.0002	0.0056	0.2430	0.0970	0.2863
	$7/2^+$	0.0001	0.0002	0.0266	0.3765	0.2207	0.3355
5	$9/2^-$	0.0000	0.0000	-0.0763	0.0680	-0.2111	0.4024
	$11/2^-$	-0.0000	0.0000	-0.0388	0.0576	-0.0641	0.3122
matching radius	kr	3		7.5		12.0	
	r	17.7		15.7		14.6	

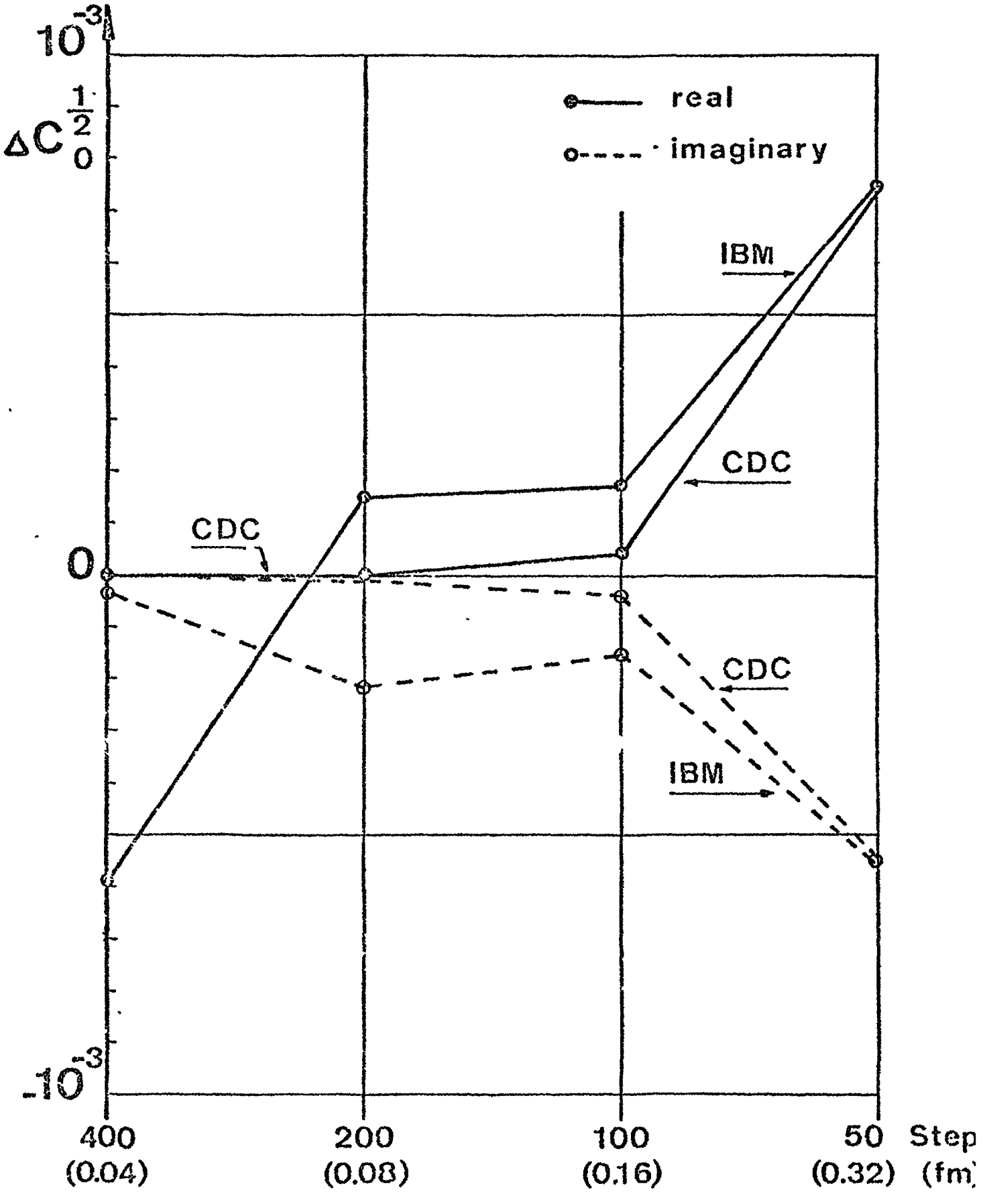

Figure 1A - The error of $C_o^{\frac{1}{2}}$ with various mesh intervals

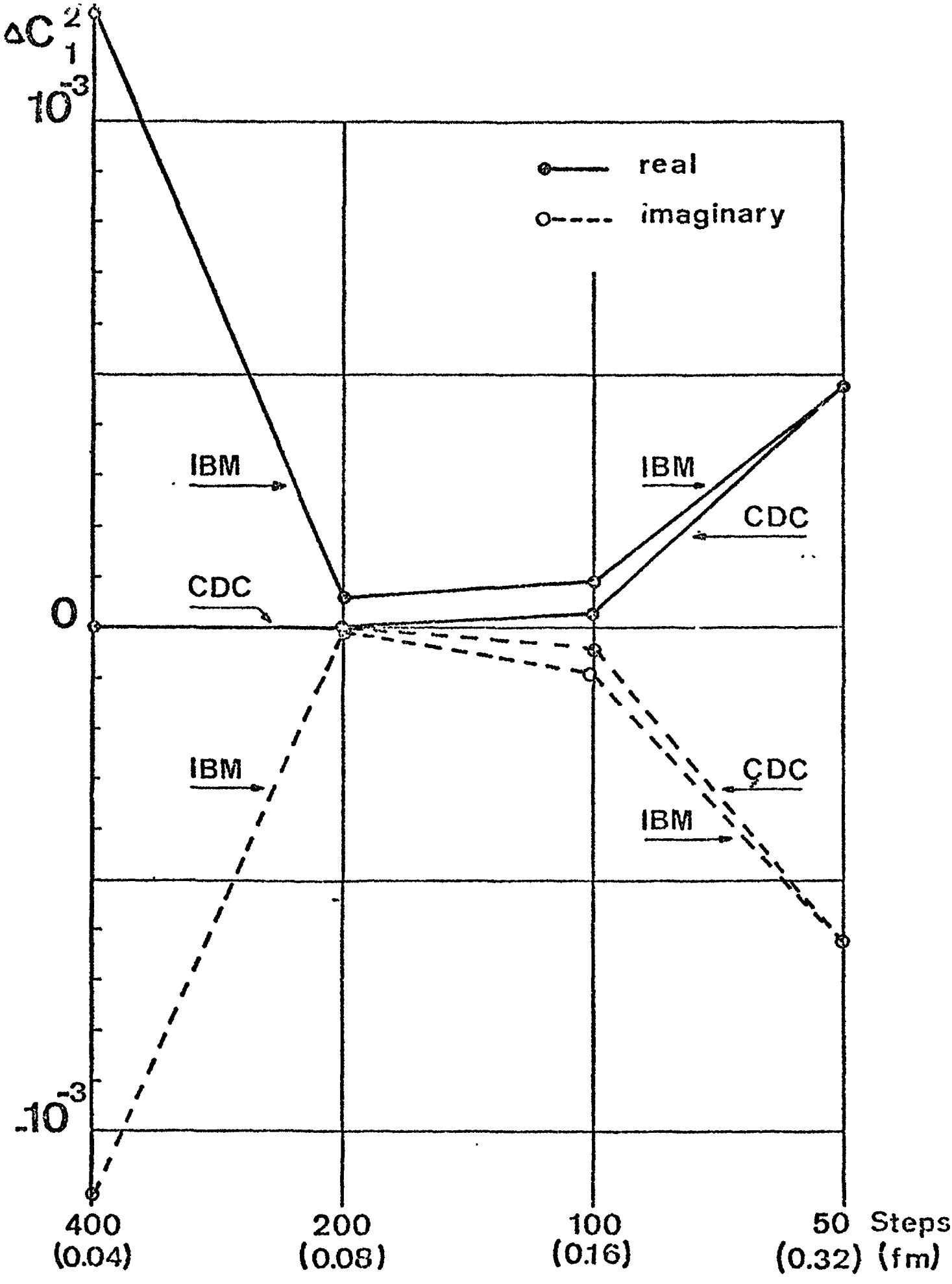

Figure 1B . The error of $C_1^{\frac{1}{2}}$ with various mesh intervals

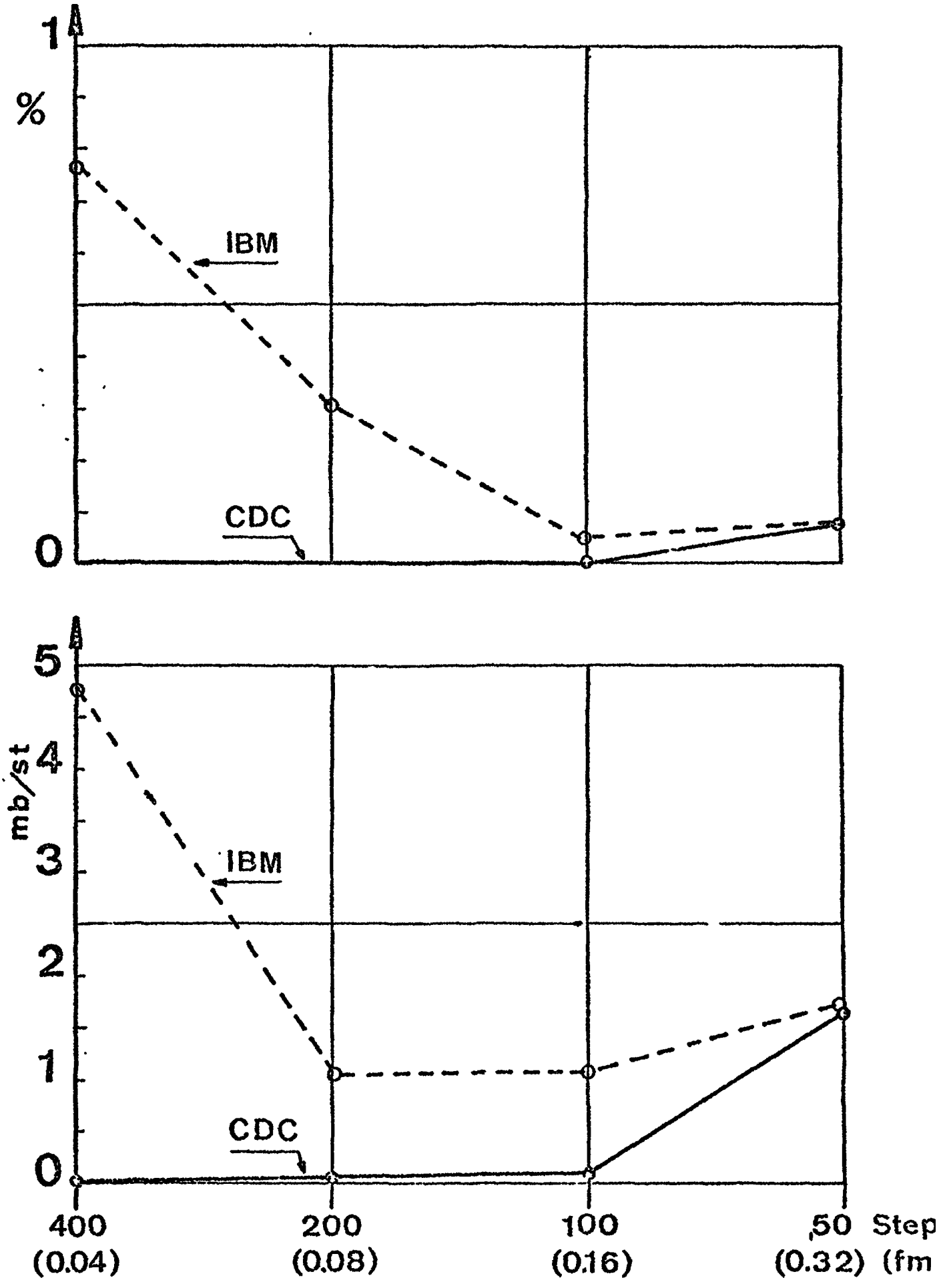

Figure 2 - The error of polarization (upside) and differential elastic scattering cross-section (downside) with various mesh intervals

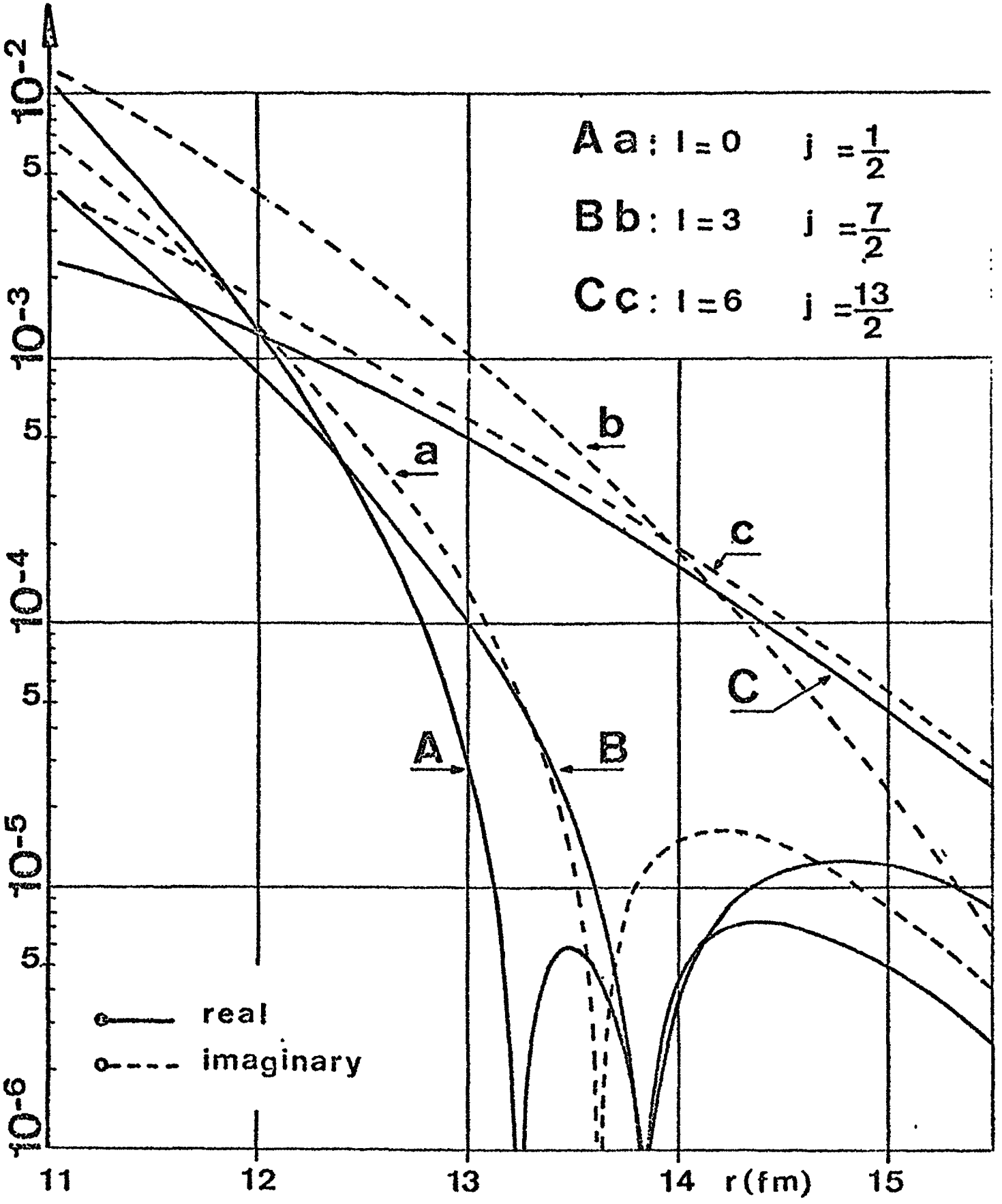

Figure 3 - $\left|c_\ell^j(r) - c_\ell^j\ (r = 18\ \text{fm})\right|$

On the Computer Codes Based on Statistical Optical and Direct Interaction Models

Sin-iti Igarasi

Abstract

This is a brief introduction of computer codes in JNDC based on statistical, optical and direct interaction models. In this report, following seven computer codes are presented; ELIESE-3, JUPITOR-1, TOTAL, RACY, STAF, TRANCE and WAFFLE. Functions of these codes are briefly represented. On ELIESE-3 and JUPITOR-1, some problems are discussed concerning with their applications.

1. Introduction

In JNDC (Japanese Nuclear Data Committee), many computer codes are prepared for the purposes of nuclear data analyses and evaluations. ELIESE-3[1] is extended from ELIESE-2[2]. JUPITOR-1[3] is a program for analyses of inelastic scattering cross-section on the basis of the coupled-channel method. TOTAL[4] is a program by which the optical potential parameters are searched for automatically over a wide range of the neutron energy. RACY[5] calculates the (n,γ) cross-section based on statistical and direct-interaction models. STAF[6] is a program for analyses of yields, angular distributions, etc. of the fission products. Other small programs are made in order to investigate some physical problems or in order to prepare the input data for other programs.

Followings are brief explanations of these computer codes. Some problems concerning with these codes are also discussed.

II. ELIESE-3

ELIESE-3 is a program which calculates the total cross-section, the compound nucleus formation cross-section, the elastic scattering cross-

section (shape and compound elastic scattering cross-sections), the polarizations of the scattered particles, the inelastic scattering cross-section, some reaction cross-sections via compound nucleus, and the angular distributions for emitted particles. Coefficients of Legendre expansion are also calculated in the center of mass system as well as the laboratory system. Calculations are applicable to the incident and emitted particles with spin 0, 1/2 and 1. The optical model, the Hauser-Feshbach and Moldauer theories are used in this program.

The optical potentials used in the ELIESE-3 are conventional local complex potential, non-local and equivalent local potentials for Gaussian and Yukawan type kernels. The potential strengths are written in the forms of second order polynomials of the energy. Automatic search for the potential parameters are possible for 1 to 15 parameters at one time.

Scattering and reactions via compound nucleus are analysed by using the Hauser-Feshbach and Moldauer theories. In the case of using the Hauser-Feshbach theory, levels in discrete and continuum regions of the residual nuclei are both available as the final states. In the case of Moldauer's theory, several lower excited states are taken as the residual states. Parameter Q which represents the resonance interference effect, is internally calculated or given as the input data. Competing processes are considered by using additional parameters, when their cross-sections or transmission coefficients cannot be calculated by the ELIESE-3.

Output data of this program are as follows.

i) The total cross-section, the compound nucleus formation cross-section, the shape and the compound elastic scattering cross-sections, angular distributions of the elastic scattering, the transmission coefficients and the coefficients of the Legendre expansion of the angular distributions.

ii) The inelastic scattering (or reaction) cross-sections, the inelastic scattering (or reaction) cross-sections to each discrete level of residual

nuclei and the angular distributions. Energy and angular distributions of the inelastic scattering (or reaction) cross-sections at each mesh point in the continuum region.

iii) The polarizations of the scattered particles, i.e. polarization, rotation and asymmetry. Tensor polarizations are added to these outputs in the case of spin 1 particles.

iv) The phase shifts of the scattered waves and the scattering amplitudes.

v) Graphic plotting is available for the angular distributions and polarizations.

Computer time estimated by the IBM 360/75 is about 0.5 to 2 sec for each discrete level or for a mesh point in the continuum region. Even in the case of iterative procedure to be needed, it is not required so much computer time.

Unrealistic change appears in the calculated inelastic scattering (or reaction) cross-section in a joint region (intermediate energy region) of discrete and continuum regions. The cross section in the intermediate energy region is calculated by using the conventional level density formula, since no information exists about discrete levels. In the intermediate region, population of the levels is not so dense as the level density formula is applicable, i.e. the level density formula gives overestimation to the population of the levels in this region. Therefore, the excitation functions for the discrete levels are abruptly decreased in the intermediate and continuum regions. This implies that some appropriate way is needed to estimate the population of the levels in the intermediate energy region. This improvement is still an open question.

III. JUPITOR-1 (Revised Version)

Program JUPITOR-1 is a revised version of T. Tamura's original program for coupled-channel. This revised program is for IBM 360/75 and FACOM 230-60

computers. Contents of the original program are completely included in the revised version. In addition to the original version, the revised one has a subroutine which calculates the integration of the angular distributions. Detailed descriptions about physical and mathematical meanings have been given in Rev. Mod. Phys. 37 679 (1965) and ORNL-4152 (1967) by T. Tamura. Then, these are not repeated here.

Followings are some remarks in the use of JUPITOR-1. In practical calculations, JUPITOR-1 has a limit in the case of non-adiabatic calculations; number of levels available is at most six. This restriction comes from saving the computer time. For heavy elements, this restriction is serious. Though adiabatic approximation can be used in this program for well deformed nuclei and high energy region, further improvement is highly desirable for wide nuclei and low energy region.

Energy dependent form of the optical potential parameters is not considered. The energy dependence of the optical potential comes mainly from coupling between entrance channel and many other channels. In JUPITOR 1, coupling between entrance channel and a few other channels is only considered. Therefore, the energy dependence of the potential parameters still remains as a result of coupling with other channels, which are not considered in the calculations. Concerning with this point as well as some other points, modification for input form of JUPITOR-1 is desirable.

There is a serious problem about relation between the spherical optical potential and the potential used in the coupled-channel calculations. For example, the inelastic scattering cross-sections are sums of ones via compound nucleus and those via channels coupled with other channels. The formers are calculated by using the Hauser-Feshbach theory or Moldauer's theory based on the spherical optical potential. The latters are obtained by the coupled-channel calculations. If both calculations were performed by the use of the same potential parameters, except for the coupling parameters β's in

the coupled-channel calculations, the total cross-sections obtained would be different with each other. Even if the different nuclear models were used, the same value of the total cross-section is, at least, a guarantee for the result of the inelastic scattering cross-sections.

IV. TOTAL

Program TOTAL is prepared for surveying the systematics of the optical potential parameters in the wide energy range of the incident neutron. Almost all of the subroutines are taken from ELIESE-3. Main control routine, input and output subroutines are revised.

Program TOTAL is able to calculate the total cross-section, the compound formation cross-section and the s-wave strength function up to a hundred energy points at one time. Automatic parameter search is performed in the same way as the ELIESE-3. Graphic plotting facilitates showing of the calculated and experimental cross-sections. Gross trend of the potential parameters is obtained by the fitting of the total cross-section. Fine systematics of the potential parameters will be looked for by the fitting of the angular distributions of the elastic scattering. This will be performed by using the ELIESE-3.

V. RACY

Program RACY is composed of RACY-S (statistical treatment) and RACY-D (direct capture and collective capture). RACY-D is used to calculate the direct capture cross-section and the collective capture cross-section. Theoretical bases of RACY-D are given by Lane-Lynn (Nucl. Phys. 11 646 (1959)), Brown (Nucl. Phys. 57 339 (1964)) and Clement et al. (Nucl. Phys. 66 272 (1965)).

Parameters concerning with the compound nucleus are the level density and a strength function for the gamma ray widths. In the program RACY, the strength function at the neutron binding energy is used as an adjustable

parameter. This parameter is determined by fitting the calculated cross-section to the experimental data at one energy. In practical calculation, the iterative procedure is used to determine the parameter.

VI. STAF

Program STAF has been developed for calculations of various quantities concerning with fission fragments, based on the statistical model. The following quantities are obtained;

i) charge distributions of the fragments,

ii) mass distributions of the fragments,

iii) total and average kinetic energies of the fragments,

iv) anisotropy of the fragment distributions,

v) average excitation energy of the fragments,

vi) average number of prompt neutrons.

Because of many kinds of integrations, this program requires long computer time. In the case of average angular momentum ≈ 3, mesh size of integration for square angular momentum ≈ 2.5 and mesh size of integration for angle ≈ 0.314 rad, it is estimated for IBM 360/75 about 4 or 5 min.

VII. Other Programs

A few small programs are prepared for calculations of some physical quantities. For examples, transmission coefficients and strength functions are calculated by TRANCE.[7] The transmission coefficients obtained are used as input data for RACY-S program. Program WAFFLE[8] shows wave functions by using the graphic plotter.

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NUCLEAR MODEL CODES USED BY THE CNEN NUCLEAR DATA GROUP

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ABSTRACT.

A brief outline of nuclear model codes used by the Nuclear Data Group of the CNEN Computing Centre (Bologna) is provided. Some of the results obtained by using different codes, approximations or computers are sometimes compared.

1. INTRODUCTION

The use of nuclear models and electronic computers for the calculation of nuclear data was started at the CNEN Computing Centre (Bologna) since the establishment of the Centre itself (July 1960). This activity was initially undertaken with the limited aim of estimating neutron capture cross-sections in the unresolved resonance region for fission product nuclei of importance for fuel cycle calculations. However, the role of the nuclear models for the evaluation work (especially in connection with the nuclear data requirements for fast reactors) was soon recognized. It was therefore decided to establish a permanent full-time group working on the development and applications of nuclear model codes. During this decennial activity various home-made codes, some of which are now obsolete, have been produced and used. Codes developed elsewhere have been used too, sometimes introducing changes to implement the codes on the computers available at the Centre.

A short account of the codes now in use is given in the following. When not otherwise stated, the programmes are written in FORTRAN IV for the IBM-7094 and/or IBM-360/75 computers.

2. STATISTICAL MODEL CODES

a) *SAUD* [1]. This code was devised in order to calculate (n,γ) cross-sections by statistical model in the framework of the Lane-Lynn formalism [2]. It was originally written for the IBM-650 and its performances are therefore rather limited. Neutron s- and p-waves only are taken into account, and the competition of the inelastic scattering with the capture process is not considered. The Porter-Thomas distribution is assumed for the reduced neutron widths of both angular momenta (ℓ=0,1). This implies numerical computations of the error-function, which in the original version (written in BELL) was approximated using a recipe given by Hasting [3]. Such an approximation does not hold whenever very small values of the strength-functions are involved. Recently, the programme has been modified in order to adopt the usual computer subroutine for the error function (IBM-360/75 version). The input parameters required are, among the others, the average radiation width, the average spacing of J=0 compound nucleus levels and the strength-functions $\bar{S}_0$, $\bar{S}_1$. The target nucleus spin I can be 0 or a half-integer up

to 9/2. Typical running times are ~0.25 sec for 20 energy points (IBM-360/75 version).

More recently (1969) a very similar programme was written by Bhat [4]. This programme, named AVERAGE, calculates not only the capture but the compound elastic scattering and fission cross-sections as well. It is written in such a way that the unresolved resonance parameters given in ENDF/B, File 2, can be fed in directly as input data. Results provided by SAUD and AVERAGE were compared at our Centre for a number of cases. It was found that the results for the $\ell=0$ component were nearly identical, but those for $\ell=1$ showed very large discrepancies. After inspection of the formulae contained in AVERAGE (version distributed by the ENEA CPL-Ispra), it turned out that the number of accessible reaction channels $\varepsilon_{j\ell}^{J}$ is probably missing in AVERAGE(1). In Table I the results of a sample calculation for ^{197}Au are shown. The adopted parameters are those of ENDF/B-II.

As one can see by comparing columns A (SAUD) and B (AVERAGE), the two programmes agree quite well for $\ell=0$, but they are strongly in disagreement for $\ell=1$. Column C shows the results obtained by introducing in AVERAGE the number of accessible reaction channels $\varepsilon_{j\ell}^{J}$. With such a modification the results given by SAUD and AVERAGE show a much closer agreement, differences being very likely due to the different methods adopted in performing the Porter-Thomas average.

b) *FISPRO* [5]. This code was written in order to quickly carry out a large amount of neutron radiative cross-section calculations. The availability of a very fast code is of primary importance when the gross behaviour of the capture cross-section for bulk fission product nuclei has to be evaluated. In such a circumstance, in fact, an estimate of several thousand cross-section values is required. The model adopted in FISPRO is essentially the Hauser-Feshbach one as developed by Margolis [6]. In addition, the code allows for a rough estimate of the cross-sections for the following processes:
i) one-photon "evaporation"
ii) two-photons "evaporation"
iii) direct and semi-direct capture.
In the last version (FISPRO-II), two different formulae can be selected for the energy dependence of Γ_γ, based on the so-called "Weisskopf" and "Axel" estimates respectively. A $(2J+1)$ law is adopted for the spin dependence of the level density.

As far as the choice of the neutron penetrabilities T_ℓ is concerned, there are three options:
1) The T_ℓ are computed according to the strong interaction model $(\ell\leq 4)$.
2) The T_ℓ are computed by means of the spherical optical model $(\ell\leq 9)$. The following optical potentials are allowed (without spin-orbit coupling): Saxon-Woods, Buck-Perey, Gauss and square-well.
3) The T_ℓ are given in input $(\ell\leq 9)$.

One of the main deficiencies of the programme is due to the fact that the Porter-Thomas distribution of the reduced neutron widths is not taken into account. In the version for the IBM-7094, typical running times range from 0.5 to 10 sec per energy point, depending on the adopted option.

For some nuclei, Gardner [7] compared the results given by FISPRO with those given by ABACUS-NEARREX. Unfortunately the adopted T_ℓ were not

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(1) In the formula for the elastic scattering a summation too seems to be missing.

the same in both cases, so that definite conclusions cannot be drawn concerning the observed differences. Cross-sections for the photon "evaporation" process in ^{127}I neutron capture were calculated by Sperber [8] and compared with those given by FISPRO. Discrepancies of about a factor three at ~5 MeV up to 2-3 order of magnitude at ~14 MeV were found, Sperber's values being always larger. These discrepancies were explained mainly in terms of the different level density formulae adopted. The formula used by Sperber, in fact, assumes a more sophisticated spin dependence than the (2J+1) one. It is not clear, however, whether or not the competition of the $(n,\gamma n')$ process is taken into account by Sperber(2). It is obvious that if such a competition is ignored, the calculated cross-sections are those for all radiative processes which, at high energies, are in general much larger than those for the capture process only.

c) *MARE* [9]. This programme was written in order to estimate the cross-sections for reactions induced by particles of several MeV kinetic energy. The theoretical background is provided by the evaporation model and the Blatt-Ewing formula. The programme gives the cross-sections for (x;a), (x;a,b), (x;a,b,n) processes, where the symbols x , a and b represent neutrons, protons, alpha or gamma rays indifferently. It is assumed that compound nucleus processes only take place and that no more than three successive particle emissions are energetically allowed. Typical running times are ~3 sec for an (x;a,b) reaction (one energy point) on the IBM-360/75.

d) *SASSI* [10]. This programme calculates the ½ spin neutron scattering cross-sections by a spherical potential with a spin-orbit term. The programme outputs are the total and reaction cross-sections, as well as the angular distributions for shape-elastic and compound nucleus processes (elastic and inelastic). The theoretical backgrounds are provided by the spherical optical model and the Hauser-Feshbach statistical model as modified by Goldmann and Lubitz [11] to include spin-orbit effects. Porter-Thomas fluctuations and competition of reactions other than (n,n) and (n,n') are not considered. In the IBM-360/75 version, angular momenta up to ℓ=50 are allowed, and the maximum number of excited levels admitted is 100. No option for automatic search for best fit parameters is provided.

SASSI is very similar to the well known ABACUS, whose numerical results have been found to be well in agreement with those given by SASSI. In Table II an example of such an agreement is given. The numerical results are those of SASSI and ABACUS-II (GE-625 version) for the sample problem reported in GEMP-447.

e) *ISOSTA* [12]. This programme was written to calculate the cross-sections for compound nucleus neutron radiative capture processes leading to isomeric states. The theoretical backgrounds are given by the Hauser-Feshbach and Huizenga-Vandenbosch [13] theories. This programme has not yet been fully tested.

3. OPTICAL MODEL CODES

a) *SMOG* [14]. The mathematical aspects of this programme, whose first version was written several years ago for the IBM-704 computer, are very similar to those of the well known SCAT programme [15]. It was included in SASSI (see above) to carry out the spherical optical model calculations required by

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(2) Our attention on this point was called by D.G. Gardner (private communication).

that programme, so that the reader can refer to SASSI for a short description of its performances.

b) *ADAPE* [16]. This programme can calculate the total cross-section and the total and differential elastic and direct inelastic scattering cross-sections for 0 or ½ spin nuclear particles from a rotational permanently deformed nucleus of either even or odd A. The theoretical background is provided by the coupled channel theory in adiabatic approximation. Numerical results were found to be in close agreement with those given by the revised version of JUPITOR (see below). Typical running times are of the order of 5 min on the IBM-7094 and ~1 min on the IBM-360/75 computer.

c) *DUMBO* [17] and *DANGFASI* [18]. These programmes, written in FORTRAN II, belong to the series of generalized optical model codes for even-even nuclei, like the 2-PLUS code written by Dunford [19].

DUMBO (1963), calculates the 0 spin neutron scattering from target even-even collective nuclei with a coupled channel method. Only the coupling between the ground state and the first 2^+ excited state of the target is taken into account. The 2^+ target level can be either of vibrational or of rotational kind. The programme outputs are constituted by the total cross-section, the reaction cross-section, the total and differential shape elastic and direct 2^+ inelastic cross-sections, the strength functions and penetrabilities. Typical running times are of the order of 1 min.

DANGFASI is an extension of DUMBO to the case of ½ spin incident neutrons. In addition, the programme calculates the elastic scattering phase-shifts as well as the polarization of the scattered neutron. Typical running times are of the order of 2 min on the IBM-7094. Numerical results agree very well with those given by 2-PLUS (see Table III-B). It has to be noted that in these two programmes the interaction potential is developed (to the first order) in powers of the deformation parameter. Such a feature must be taken into account whenever comparing numerical results of DUMBO and DANGFASI with those given by other programmes using a Legendre polynomial expansion.

d) *"JUPITOR"*. A version of the JUPITOR code [20] for CDC computers, kindly provided to the CNEN Computing Centre by the author T. Tamura, was checked [3] in almost all its parts and implemented [3] for the IBM-7094 and IBM-360/75 computers. Several clerical errors were found and some incompatibilities between CDC and IBM FORTRAN languages were removed. As stated above, the numerical results obtained whenever the adiabatic approximation is used are in very good agreement with the results given by ADAPE. An example is given in Table III-A, where results of ADAPE and "JUPITOR" are compared for the case of 7.5 MeV neutrons scattered by ^{165}Ho.

The following set of parameters was adopted:

$$\left.\begin{aligned} V &= 45.5 \\ W_D &= 5.75 \\ V_{SO} &= 10 \end{aligned}\right\} \text{ MeV} \qquad \left.\begin{aligned} a_V &= a_{VSO} = 0.58 \\ a_{WD} &= 0.35 \\ r_{OV} &= r_{OWD} = r_{OVSO} = 1.25 \end{aligned}\right\} \text{ fm}$$

with β=0.30 and $\ell_{max} = 8$. The adopted level spins and parities were $7/2^+$, $9/2^+$, $11/2^+$.

To further test the code, calculations were carried out assuming the

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(3) By F. Fabbri and P.L. Ottaviani.

deformation parameter $\beta=0$. In this way the optical potential is reduced to the spherical one, and it is therefore possible to compare the numerical results obtained with those given by other codes. Table III-B provides an example of such a comparison among the codes SASSI, 2-PLUS and "JUPITOR". The calculated cross-sections are those for 1 MeV neutrons interacting with ^{184}W. The adopted parameters were:

$$\left.\begin{array}{l} V = 45.05 \\ W_D = 6.68 \\ V_{SO} = 6.20 \end{array}\right\} \text{MeV} \qquad \left.\begin{array}{l} a_V = a_{VSO} = 0.65 \\ a_{WD} = 0.47 \\ r_{OV} = r_{OWD} = r_{OVSO} = 1.25 \end{array}\right\} \text{fm}$$

with $\ell_{max} = 5$.

The adopted level scheme was: $0,(0^+)$; $0.111(2^+)$; $0.364(4^+)$; $0.750(6^+)$; $0.904(2^+)$.

In Table III-B a comparison among 2-PLUS, "JUPITOR" and DANGFASI for the same case but with $\beta=0.24$ is also shown. The rotor model was assumed, with a deformed potential developed in powers of β up to the first order. Obviously, only the coupling $(0^+,2^+)$ was considered in "JUPITOR". The small differences among the numerical results are almost entirely due to the fact that "JUPITOR" uses an integration method with variable mesh, whereas in 2-PLUS and DANGFASI a fixed mesh method is adopted.

4. DIRECT INTERACTION CODES

a) *DIRCO* [21]. This programme calculates the dipole radiative capture of nucleons by nuclei in the framework of the "direct" and "collective" models. In particular, the direct and collective capture cross-sections for individual single-particle bound states are calculated for a given incident nucleon energy. The total cross-section is then given as the sum of the contributions over all possible final states. The incident particle and the target nucleus are assumed to interact through a spherical optical potential including the spin-orbit interaction. The target nucleus is assumed to have zero-spin. The interference between the two capture processes is taken into account in the calculations. The programme has a vast flexibility as to the shape of the interaction that can be used. The programme outputs are the cross-sections and the radial integrals for individual transitions. Optionally, cross-sections (total, direct, collective and interference), wavefunctions, and radial integral squares can be plotted vs. the incident nucleon energy.

b) *KISS* [22]. This code was written to calculate the cross-section for quadrupole direct radiative capture of nucleons by nuclei. Its performances and outputs are very similar to those of DIRCO.

c) *PRODE* [23]. This code calculates the cross-section for direct (n,p) reactions. The physical background is given by the Brown-Muirhead [24] model, which assumes a Fermi-gas representation of the nucleus. The programme calculates the probability that a proton is knocked-out by the impinging neutron without further collisions. From this probability, the cross-section for the (volume) direct (n,p) reaction is easily obtained. The outputs are the cross-section as well as the energy distribution of the emitted protons. Typical running times are ~0.5 sec for one energy point on the IBM-360/75.

5. MICROSCOPIC MODEL CODES

a) *SURF* [25]. The output data of this programme are the dipole photoreaction cross-sections of doubly closed shell nuclei in the one particle-one hole continuum approximation. The Schrödinger equation of the system is solved in the coordinate space by means of the coupled-channel method, taking into account the isospin mixing between the T=1 and T=0 states.

b) *MIDI* [26]. The programme calculates the dipole radiative capture cross-sections of nucleons by even-even nuclei using a coupled-channel method. The model assumes that the incident nucleon interacts with the target through a Woods-Saxon potential taking into account the target excitations in the giant resonance region. The spectrum of the target can be described by means of a collective model (phonon excitations) or by a microscopic model (1p-1h excitations in Tamm-Dancoff or RPA approximation).

c) *MIMOC* [27]. The code can calculate the elastic scattering phase-shifts and cross-sections for incident nucleons on even-even nuclei with a microscopic description of target states. The wave-equation is solved in the framework of the coupled-channel theory.

d) *RES* [28]. This programme allows to extract the spectroscopic parameters (resonance energy, total and partial widths, configuration mixing coefficients) of a resonant cross-section calculated using a microscopic coupled-channel model.

e) *JUPITOR MICRO* [29]. Tamura's JUPITOR code was extended to the case of odd-deformed nuclei to allow for the presence of several rotational bands. A nuclear level of given angular momentum is described as a sum of nuclear levels of equal angular momentum belonging to different bands (band-mixing). The excitation of rotational bands other than the fundamental one is obtained, even in absence of band mixing, by introducing a microscopic nucleon-nucleon interaction allowing the transition of the bound odd nucleon to different orbits. The different intrinsic levels of the various bands are thus generated. Space-exchange effects between the projectile and the odd-target nucleon are ignored.

6. MISCELLANEA

Many auxiliary programmes developed at the CNEN Computing Centre are strictly connected with the use and development of nuclear model codes. Among the others, it is worthwhile mentioning the following:

a) *SPEC* [30]. It calculates the γ-ray spectra from radiative nucleon capture reactions in the MeV nucleon energy range according to direct and collective mechanisms. To compare calculated and measured spectra, the programme relies on DIRCO to calculate the cross-sections spreading them over an energy interval corresponding to the resolution of the spectrometer.

b) *LILABNER* [31]. Calculating the level density parameter a of the Fermi-gas model. Eight different expressions of the level density formula are considered by the programme.

c) *FGETA* [32]. This subroutine calculates the regular and irregular Coulomb functions and their derivatives.

d) *BOSTAW* [33]. The programme calculates the normalized eigenfunctions for a nucleon bound in a Woods-Saxon well. If the potential well is known, the programme provides the eigenvalues and viceversa.

e) *RAFF* [34]. Radial form factors suitable for inelastic scattering calculations can be obtained through this programme. The single-particle wave functions used in the calculations may be eigenstates either of a Woods-Saxon potential well or of an oscillator potential well. Gaussian, Yukawa or Coulomb radial dependence can be used for the two-body interaction.

f) *EXODUS* [35]. An IBM-360 system code analysing inelastic scattering continuum spectra on the basis of H.F. theory. The code takes advantage of the IBM-2250 Display Unit. By using SASSI, the code calculates:

- the usual quantities of the (spherical) optical model;
- the excitation functions of the various levels in the framework of the conventional H.F. theory;
- a gaussian convolution of groups of inelastic differential cross-sections at a given angle.

The average cross-sections observed are thus simulated. The results of the calculation are plotted on the Display Unit, together with the experimental data. Through a conversative interaction, it is possible to modify:
i) the optical model parameters;
ii) the target nucleus level scheme (energies, spins and parities);
until a reasonable fit is achieved for the experimental data. As an example, the figure shows the results of a preliminary analysis of the Perey-Kinney data at 8.56 MeV for ^{23}Na (ORNL-4518). At this incident neutron energy more than 50 levels can be excited; for most of them, however, the spin and parity assignment is unknown. The experimental data refer to 90° degrees in the Lab. system and are in unit of mb/sr/25 keV. The energy spread is approximately gaussian with ~160 keV F.W.H.M. - The excitation energy of the residual nucleus ranges from ~5.5 MeV up to ~7 MeV.

Picture a) shows the theoretical result (continuous curve)obtained by assuming an arbitrary spin and parity assignment for the unknown levels. Picture b) shows the final result, after the unknown quantities have been selected on the basis of a trial- and error procedure. Both pictures have been obtained directly by taking a photograph of the D.U. screen.

g) *NILSSON* [36]. This programme calculates the eigenvalues and the eigenfunctions of the hamiltonian of a single $\frac{1}{2}$ spin particle subject to a Nilsson potential, i.e. an axially deformed harmonic oscillator potential plus $\underline{\ell}.\underline{s}$ and $\underline{\ell}.\underline{\ell}$ contributions. As in Nilsson's work, the representation chosen for the diagonalization of the total hamiltonian is the isotropic-oscillator one where ℓ^2 and ℓ_z, s_z (the orbital and spin angular momentum components along the axis of symmetry) are diagonal. However, the eigenfunctions are also expressed in the representation where the total angular momentum $\underline{j}=\underline{\ell}+\underline{s}$ and its component along the axis of symmetry j_z are diagonal. Major shell mixing is allowed. For each orbit the intrinsic quadrupole moment, the mean value of the potential and of r^2, r^4, $r^4Y_2^0(\theta)$ as well as the orbital density, are calculated. The decoupling parameter is calculated for orbits having the component of j_z equal to $\frac{1}{2}$. The programme can also be used to study the properties of different intrinsic states of a nucleus. For each single combination of occupied levels the total energy, the intrinsic quadrupole moment of the matter distribution, the mean value of r^2, r^4, $r^4Y_2^0(\theta)$ are calculated, along with the density, if requested.

Performing the calculation for different values of the potential deformation, the energy minimum and the equilibrium deformation of each intrinsic state can be found.

7. CONCLUSIVE REMARKS

The main features of the nuclear model codes in use at the CNEN Computing Centre are summarized in Table IV. In spite of the fact that these codes appear to be useful in the study of a number of problems, it is clear that a substantial effort is still necessary in order to face the various needs of the nuclear data evaluation work. For example, no codes dealing with the fission process have yet been developed or used by the Nuclear Data Group, and no self-consistent, comprehensive nuclear theory calculation system is, as of now, available at the Bologna Centre.

Last, but not least, it should be noted that the nuclear model codes are of little use if they are not supported by good sets of parameters. A large amount of analyses is still necessary in this field to improve the present unsatisfactory situation.

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TABLE I

A comparison between SAUD and AVERAGE for ^{197}Au

En (keV) \ σ(n,γ) (barn)	ℓ = 0		ℓ = 1		
	A	B	A	B	C
1	7.849	7.875	0.148	0.109	0.163
2	4.392	4.404	0.248	0.151	0.226
3	3.106	3.113	0.295	0.181	0.271
4	3.422	3.428	0.331	0.204	0.305
5	1.994	2.000	0.358	0.222	0.333
6	1.700	1.703	0.379	0.237	0.354
7	1.483	1.482	0.396	0.249	0.372
8	1.318	1.321	0.410	0.259	0.387
9	1.187	1.190	0.421	0.267	0.399
10	1.081	1.083	0.429	0.274	0.409

TABLE II

A comparison between SASSI and ABACUS-II (Sample problem)

Quantity (barn)	SASSI (IBM-7094)	ABACUS-II (GE-625)
σ_T	5.615	5.6149
$\sigma_{s.el.}$	3.221	3.2208
σ_R	2.394	2.3941
$\sigma_{s.el.}$ (0°)	1.5720438	1.5721
$\sigma_{s.el.}$ (90°)	0.0780441	0.07843
$\sigma_{s.el.}$ (180°)	0.1233591	0.12336
$\sigma_{c.el.}$ (0°)	0.0866189	0.0867005
$\sigma_{c.el.}$ (90°)	0.0634759	0.0635335

TABLE III-A

A comparison between ADAPE and "JUPITOR" for ^{165}Ho

Quantity (barn)	ADAPE		"JUPITOR"	
	IBM-7094	IBM-360/75	IBM-7094	IBM-360/75
σ_T	4.905742	4.909581	4.90773	4.90756
$\sigma_{s.el.}$	2.452888	2.446848	2.48620	2.48610
$\sigma_{d.in.}$ (9/2)	0.274836	0.275864	0.27559	0.27563
$\sigma_{d.in.}$ (11/2)	0.120244	0.121650	0.12127	0.12162

TABLE III-B

A comparison among SASSI, 2-PLUS, DANGFASI and "JUPITOR" for spherical and non-spherical cases

Quantity (barn)	SASSI	2-PLUS (β=0)	"JUPITOR" (β=0)	2-PLUS (β=0.24)	"JUPITOR" (β=0.24)	DANGFASI (β=0.24)
σ_T	7.2782	7.2763	7.2947	6.6632	6.6724	6.6645
σ_R	3.4566	3.4541	3.4673	3.2068	3.1986	3.2055
σ_{se}	3.8216	3.8222	3.8274	3.4564	3.4738	3.4590
σ_{ce}	0.7950	0.7947	0.7975	0.7582	0.7695	-
σ_{ci} (1°)	1.8105	1.8095	1.8172	1.4766	1.4787	-
σ_{ci} (2°)	0.4154	0.4149	0.4162	0.3783	0.3805	-
σ_{ci} (3°)	0.0023	0.0023	0.0023	0.0021	0.0021	-
σ_{ci} (4°)	0.4334	0.4337	0.4341	0.3549	0.3575	-
σ_{ci} (total)	2.6616	2.6594	2.6699	2.2119	2.2188	-
$\sigma_{dir.inel.}$	-	-	-	0.2367	0.2367	0.2367

TABLE IV

Nuclear model code in use at the CNEN Computing Centre

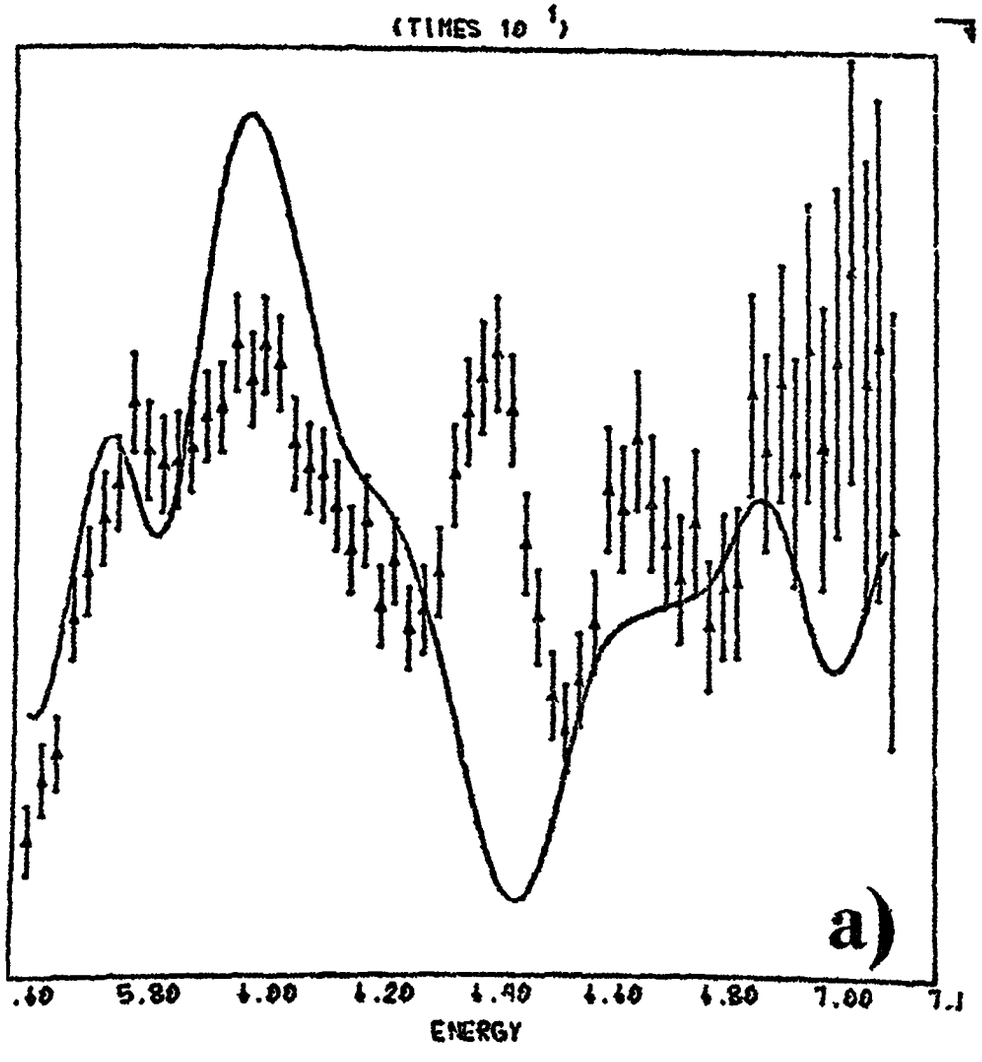
Name	Comments	CT[(a)]	W.U.?[(b)]	CPL?[(c)]	COMP?[(d)]
	A) *STATISTICAL MODEL CODES*				
SAUD	$\sigma(n,\gamma)$ by Lane-Lynn method; no competition by (n,n') or other processes; $\ell=0,1$	A;B	yes	yes	yes
FISPRO	$\sigma(n,\gamma)$ by H.F. theory; competition by (n,n') only; no fluctuations; $\ell\leq 9$	A;B	yes	yes	yes
MARE	$\sigma(x;a)$; $\sigma(x,a,b)$, $\sigma(x;a,b,n)$; $(x,a,b)\rightarrow(n,p,\alpha,\gamma)$; evaporation model	A;B	in press	no	no
SASSI	$\sigma(n,n')$ by H.F. theory; no fluctuations or competition by other processes, $\ell\leq 50$	A;B	yes	yes	yes
ISOSTA	$\sigma(n,\gamma)$ for isomeric states; H.F. + Huizenga-Vandenbosch model	A	no	no	no
	B) *OPTICAL MODEL CODES*				
SMOG	Spherical o.m.; many types of potential are possible	A;B	yes	yes	yes
ADAPE	Deformed o.m.; adiabatic approximation	A;B	yes	no	yes
DUMBO	$\sigma(n,n)$, $\sigma(n,n')$ for $2^+\rightarrow 0^+$ transitions in deformed nuclei; no spin orbit coupling	A	yes	yes	yes
DANGFASI	As DUMBO + phase shift analysis; spin-orbit coupling	A	yes	yes	yes
"JUPITOR"	Revised version of JUPITOR1 in use at the CNEN Computing Centre	A;B	no	yes	yes
	C) *DIRECT INTERACTION CODES*				
DIRCO	Dipole direct-collective $\sigma(n,\gamma)$, $\sigma(p,\gamma)$ with interference; plotter optional	A;B	in press	no	no
KISS	Quadrupole direct $\sigma(n,\gamma)$, $\sigma(p,\gamma)$; plotter optional	A;B	in press	no	no
PRODE	Direct $\sigma(n,p)$ based on Fermi-gas model; energy spectrum of protons	A;B	no	no	no

(continues)

TABLE IV (continued)

Name	Comments	CT[a]	W.U.?[b]	CPL?[c]	COMP?[d]
	D) *MICROSCOPIC MODEL CODES*				
SURF	σ_γ for doubly closed-shell nuclei; isospin mixing	A;B	yes	no	no
MIDI	Dipole $\sigma(N,\gamma)$ for e-e nuclei; coupled channel method	A;B	no	no	no
MIMOC	$\sigma(N,N)$ and phase shift for e-e nuclei	A	yes	no	no
RES	Extraction of res. spectroscopic parameters; coupled-channel method	A;B	no	no	no
JUP.MICRO	$\sigma(N,N)$; $\sigma(N,N')$; nucleon-nucleon interaction + collective potential	A	no	no	no
	E) *MISCELLANEA*				
SPEC	γ-ray spectra from direct and collective capture	A;B	in press	no	no
LILABNER	Level density parameter a of Fermi-gas model; eight options	A	no	no	no
FGETA	Regular and irregular Coulomb functions and derivatives	A;B	yes	no	no
BOSTAW	Eigenvalues or eigenfunctions for a nucleon bound in a W.S. well	A;B	yes	no	no
RAFF	Radial form factors for microscopic model calculations	A	yes	no	no
EXODUS	(n,n') spectra analysis; H.F. theory; up to 100 exct. lvls.; Display Unit required	B	no	no	no
NILSSON	Eigenvalues or eigenfunctions for a nucleon bound in a Nilsson potential	B	no	no	no

a) IBM computers for which the programme has been developed: A = IBM 7094; B = IBM 360/75; b) W.U. = write up available;
c) Availability through ENEA Programme Library - Ispra; d) COMP = compared with similar codes.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5.80
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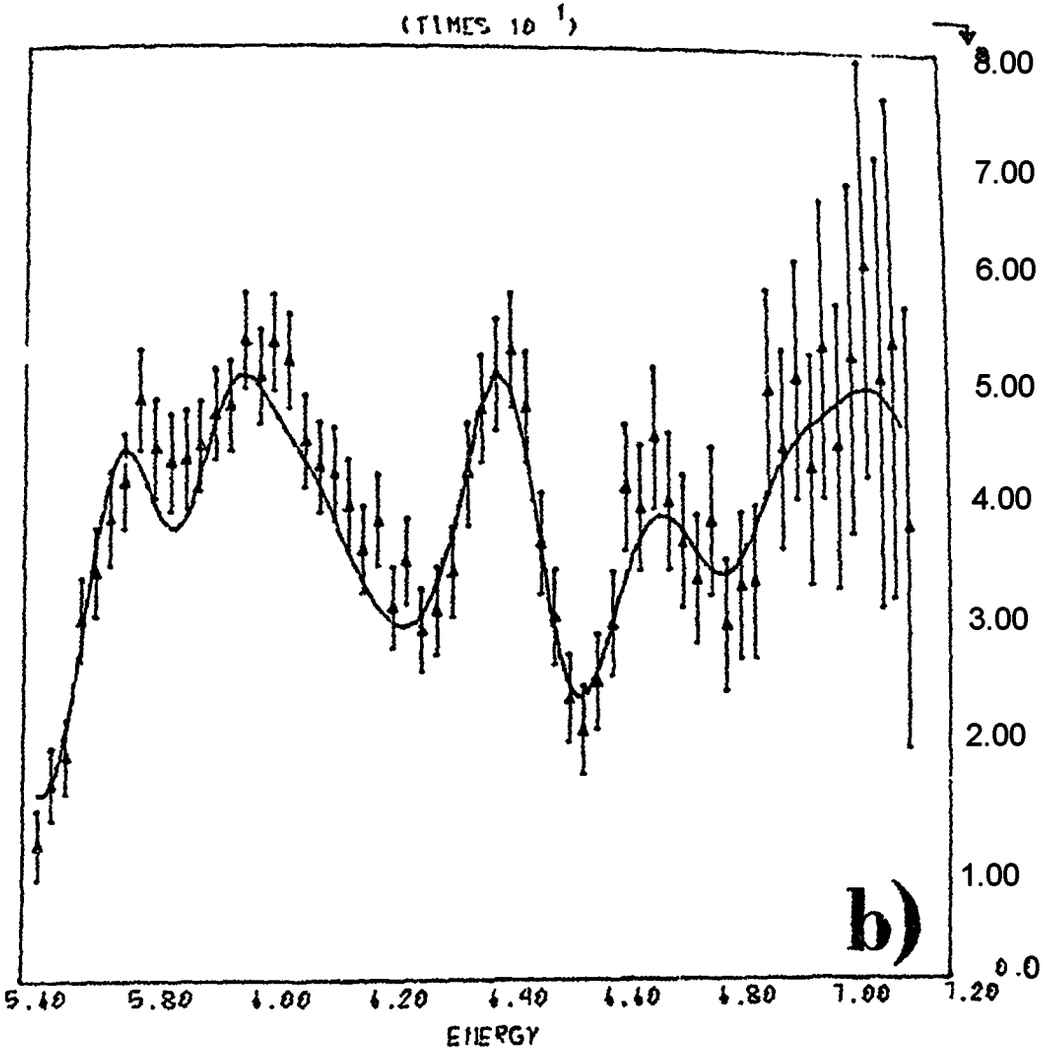
4.20
4.40
4.60
4.80
7.00
ENERGY


(TIMES 10 ⁴)
b)
8.00
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.0
5.40
5.80
4.00
4.20
4.40
4.60
4.80
7.00
1.20
ENERGY

"Notes on the Availability, Quality and Comparison of Nuclear Model Codes"

by V. Benzi

Abstract

The paper briefly sets forth a number of points which should be considered in examining the quality, availability of and comparison of computer codes used for the calculation of neutron cross sections.

The Provisional Agenda of the Panel, under item 5-II considers the following subjects:

A. *Availability, quality of and estimated computer time for computer codes.*

B. *Physical adequacy and convenience of data representation.*

C. *Comparison of computer codes - possible reasons for discrepant results.*

In accordance with the above subjects, a certain number of points ought to be taken into consideration.

i) *Availability.* A list of existing model codes should be prepared, subdivided according to the model adopted (e.g.: Spherical optical model, statistical model, etc.). Such a list should be an up-dating of the tables provided in the paper "A Brief Outline of Methods of Calculation of Neutron Cross-sections" by M.F. James (ENEA Computer Programme Library - 1966). See Annex I for a specimen.

ii) *Quality.* Whenever possible, a short comment concerning the codes appearing in the above mentioned list should be provided with regard to the flexibility (e.g., types of optical potential allowed) and the degree of sophistication (spin-orbit coupling, Porter-Thomas corrections, etc.).

iii) *Computer time.* Sufficient material will hopefully be presented by the experts allowing some conclusions about this subject.

iv) *Physical adequacy.* The limits of applicability of the various models should be discussed from the point of view of those aspects which are relevant for evaluation purposes. The status of the systematics of the parameters required by the models should also be considered. An

estimate of the confidence limits of the theoretical results would be of great importance. The feasibility of the "Pearlstein experiment" should be discussed in this context (See Annex II).

v) *Convenience of data representation*. The term "convenience" is referred to evaluation needs. In particular, the role of Display Units and conversative interactions should be examined.

vi) *Comparison of computer codes - possible reasons for discrepant results*. Here again, as for point iii), some material will hopefully be presented by the experts. Among the possible reasons for discrepant results, the following should be examined:

a) Computer used.

b) Physical limits adopted (e.g., R_{max} , l_{max} , etc.).

c) Numerical methods.

d) Fundamental constants (e.g., neutron mass).

The possibility of some concerted effort on international basis to test the various codes should also be considered.

ANNEX I

TABLE 4. PROGRAMMES FOR USE IN THE OPTICAL MODEL REGION. (A) OPTICAL MODEL PROGRAMMES

NAME	AUTHOR (S)	COMMENTS	IN LIBRARY?
ABACUS 2	AUERBACH, BNL, U.S.A.	Combined optical model and Hauser-Feshbach calculations. Includes a fitting procedure.	
OPW	WILMORE, HARWELL, U.K.	Includes a fast search routine for parameter fitting; will calculate equivalent local potential from nonlocal parameters.	Will be sent
2 PLUS	LUBITZ? KAPL, U.S.A.	Considers a deformed (non-spherical) nucleus, but only considers $2^+ \rightarrow 0^+$ transitions. May be available through DUNFORD, of Atomics International.	
SUEZ	BENZI, PANINI, ZUFFI } CNEN Bologna Italy	Assumes a square well potential.	
SMOG	BENZI, FABBRI, SARUIS } CNEN Bologna Italy	Many types of potential are possible.	Yes
DUMBO	FABBRI, SARUIS } CNEN Bologna Italy	(n,n),(n,n^1) and reaction cross-sections for $2^+ \rightarrow 0^+$ transitions in a deformed nucleus. No spin-orbit coupling.	Yes
DANG	FABBRI, SARUIS } CNEN Bologna Italy		Yes
ELIESE 1	Japanese Nuclear Data Committee, Japan	Optical model + Hauser-Feshbach theory. Calculates (n,n), (n,n^1), (n,p) and compound formation cross-sections.	
ELIESE 2	Japanese Nuclear Data Committee, Japan	As ELIESE-1, but with automatic search routine; and ability to calculate (n,α) cross-sections.	
Optical Model Parameter Search 64	HILL, Oxford University U.K.	In Atlas Autocode. Probably very similar to OPW+HFW. See BNL9108, page 39.	
INS AND ELASTIC SCAT	MITSUJI KAWAI, Tokyo Institute of Technology, Japan	Calculation of differential cross-sections of (n,n) and of polarization of scattered neutrons. See BNL9108, page 47.	

ANNEX II

PROPOSAL FOR A "PEARLSTEIN EXPERIMENT"

V. Benzi

During the AEC-ENEA Seminar on Evaluation, held at Brookhaven in 1965, in summarizing one of the Seminar Sections, S. Pearlstein stated: *"I would like to share one experience with you that is related to the work of the evaluator. Three weeks ago an engineer came into my office to say 'Because you are an expert in neutron cross-sections, I want to ask you a question'. I am going to ask you the same question he asked me since you are experts in neutron cross-sections too. The question is: 'Can you give me the cross-section information I need to know for a nucleus that has not been measured if I give you two facts, the atomic number and the atomic mass?'"* After some comments on how life is, Pearlstein concluded: *"In essence he was asking whether we have observed sufficient systematic behaviour among nuclei that would enable us to predict with confidence cross-sections where measurements have not been performed. So I think it was a fair question".*

In the last years some improvement has been obtained both in modelistic and systematics. However, a large degree of arbitrariness still exists in selecting models and parameters whenever a theoretical estimate of an unmeasured cross-section is required. For this reason, it seems it would be interesting to compare the results obtained by evaluators from different Laboratories estimating the unknown cross-sections of a given nucleus. Such a comparison should provide us with some feelings concerning the degree of convergence (or divergence) obtainable whenever evaluating cross-sections on almost purely theoretical basis.

Calculations should be carried out over the 1 keV÷15 MeV energy range.

Volunteers should be asked, on a world-wide basis, to produce a model-evaluated data file together with a report describing the models and parameters adopted. An informal final report comparing the obtained results should be compiled (for instance, by the NDS-IAEA).

The Xe-135 nucleus seems to be appropriate for such an experiment. In fact, Xe-135 is an important nucleus for reactor calculations, but only the total cross-section below 0.5 eV has so far been measured (see CINDA 71).

I. Fast Neutron Cross Sections of Elemental Titanium Microscopic Measurement and Interpretation

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ABSTRACT

Neutron total, and elastic- and inelastic-scattering cross sections of natural titanium were measured. Total cross sections were determined over the interval 0.1 to 1.5 MeV with resolutions of $\gtrsim$ 1.5 keV. Differential elastic and inelastic neutron scattering angular distributions were measured from 0.3 to 1.5 MeV with resolutions of $\gtrsim$ 5 keV. The cross sections for the inelastic neutron excitation of states in ^{46}Ti (889.2 keV), ^{48}Ti (983.5 keV) and ^{47}Ti (159.6 keV) were determined. The energy-averaged behavior of the measured results was described in terms of optical- and statistical-models.

A. Introduction

It was the objective of this work to; a) provide a detailed and internally consistent set of experimental fast neutron cross sections of titanium specifically meeting requests for basic data[1] and providing a foundation for thorough evaluation, and b) test the validity of nuclear

models and reaction mechanisms with particular attention to the concurrent description of a number of facets of the neutron-nucleus interaction.

The isotopes of titanium lie near the 3S peak of the $\ell = 0$ strength function distribution.[2] The measured strength functions in this region have been well described by selected optical-potentials[3] but the description of measured partial neutron cross sections at higher incident energies is uncertain due, in part, to a lack of detailed experimental information. Reported fast neutron total neutron cross sections of titanium display considerable structure well into the MeV region.[4] Physical understanding of this structure is not unambiguous. The even-isotopes of titanium are known to be deformed with collective-vibrational (2+) first excited states.[5] Inelastic neutron excitation of these states can be experimentally observed with a precision suitable for a quantitative assay of the effects of deformation on neutron processes at energies of one MeV and above. This study relates to all of these physical characteristics.

B. Experimental Method

The total, elastic-scattering and broad-resolution inelastic-scattering neutron cross sections were measured at Argonne. Fine resolution inelastic-scattering neutron cross section measurements were made at Pelindaba. The methods employed at both laboratories have been extensively described elsewhere and will not be further defined herein.[6,7,8] The total cross section values were deduced from transmission measurements. All scattering measurements were made relative to the known differential elastic scattering cross sections of carbon.[9] Where appropriate, "in-scattering," multiple-scattering and beam attenuation corrections were applied to the measured values. These corrections were generally small. The measurements were made using high-purity samples of the natural element. All measured cross sections are expressed in units of barns referenced to the natural element.

C. Experimental Results

1. Total Neutron Cross Sections

Total neutron cross sections were determined from 0.1 to 0.45 MeV and from 1.025 to 1.475 MeV with incident energy resolutions of $\lesssim$ 2.0 keV. From 0.45 to 1.025 MeV the experimental velocity resolution was $\approx$ 0.01 nsec/meter. The absolute energy scale was determined from known reaction thresholds, for example, $Li^7(p,n)Be^7$,[10] and from a comparison of neutron velocity with that of light. The absolute energy scale was believed known to within $\lesssim$ 8 keV. The experimental results, summarized in Fig. 1, were consistent with previously reported values[4] but displayed a great deal more structure due to improved experimental resolution. Resonances were evidently interferring when from a single isotope, overlapping when from various isotopes and merged when averaged to give the appearance of an intermediate resonance structure.[11]

2. Elastic Scattering Cross Sections

Differential elastic scattering cross sections were measured at incident neutron energies from 0.3 to 1.5 MeV and at eight scattering angles approximately equally distributed between 25 and 155 degrees. The incident neutron energy resolution was $\sim$ 20 keV. The measured differential cross sections were least-square fitted with the expression

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi}\left[1 + \sum_{n=1}^{4} \omega_n P_n\right] \qquad (1)$$

where σ (elastic cross section) and ω_n coefficients were obtained from the fitting procedure and P_n were Legendre polynomials expressed in the laboratory coordinate system. The uncertainties in the individual differential cross section values were $\lesssim$ 10%. The "goodness" of the fit was indicated by the uncertainties in the respective ω_n coefficients deduced from the fitting procedures.

The experimental elastic scattering results are summarized in Figs. 2, 3 and 4. They are relatively consistent with the measured total neutron cross sections when the different energy resolutions and small variations in absolute energy scale are considered as shown in Fig. 1. Comparable previous measurements of elastic scattering from titanium are largely confined to energies near 1.0 MeV.[12,13,14] These are compared with the results of the present work in Fig. 3. The agreement with the results of Walt and Barschall[12] is good. Below the inelastic thresholds the present elastic scattering values are consistent with the total neutron scattering distributions reported by Langsdorf et al.[9] The agreement with the values of Refs. 13 and 14 is less satisfactory.

3. Inelastic Neutron Scattering Cross Sections

Natural titanium consists of the isotopes 46 (7.93%), 47 (7.28%), 48 (73.94%), 49 (5.51%) and 50 (5.34%).[5] Of these titanium 46, 47 and 48 made the major inelastic contributions in the present work. The inelastic neutron excitation of states at 889.2 $\pm$ .2 and 983.5 $\pm$ 0.2 keV was clearly observed and attributed to known 2+ states in titanium -46 and -48, respectively.[5] In addition the excitation of a 159.6 $\pm$ 2 keV state was observed and associated with the reported 160 keV ($\frac{7}{2}$ -) state of titanium -47. The energy scales were established by careful observation of gamma-rays emitted subsequent to inelastic neutron scattering.[15] Cross sections were determined for the excitation of the 889.2 and 983.5 keV states. Those of the 159.6 keV state were small (< 3 mb/sr).

The angular distributions of inelastically scattered neutrons were determined with incident neutron resolutions of $\sim$ 20 keV. Generally these distributions were isotropic to within the experimental uncertainties as shown in Fig. 4. Differential inelastic cross sections were determined with "fine" incident resolutions (5 to 10 keV) at a scattering angle of ninety

degrees. In view of the observed isotropy, the inelastic excitation cross sections were obtained from the averaged angular distribution measurements or fine resolution ninety degree values by multiplying the averaged values by 4π. The results are summarized in Fig. 5. The broad and the fine resolution results are relatively consistent though the latter show appreciably more structure. The illustrated uncertainties in the measured cross sections were obtained from subjective estimates of the cumulative errors inclusive of; statistical uncertainties, the effects of experimental resolutions and backgrounds and uncertainties in the carbon reference standard.

Previously reported inelastic cross sections of titanium in the energy region of the present experiment are sparse. However, the results obtained by Beyster and Walt near 1.0 MeV using threshold techniques are consistent with the total inelastic cross section deduced from the present work.[16]

D. Interpretation and Discussion

The experimental values were compared with those calculated from optical-model and statistical theories.[17,18] The majority of the calculations employed a spherical potential consisting of; a Saxon-Woods real form, a Gaussian surface-imaginary form and a Thomas spin-orbit term.[17] Non-locality was approximated with energy dependent parameters.[19] The effects of deformation and direct reactions were assayed using a non-spherical optical potential inclusive of two-channel coupling to the first excited state of the even nuclei.[20]

An initial estimate of potential parameters was obtained from a comparison of measured and calculated total neutron cross sections.[21] Subsequently, small adjustements were made to give improved agreement with the measured elastic angular distributions. The resulting "selected" parameters,

given in Table 1, were based entirely upon comparisons with the present experimental results. The parameter selection was by subjective judgement. Numerical procedures, such as χ_i-squared fitting, led to parameters strongly associated with energy-local structure and not representative of the entire experimental energy range. The total neutron cross sections calculated from the spherical potential and parameters of Table 1 were descriptive of the energy-averaged experimental total and angle-integrated elastic cross sections as indicated in Fig. 1. The agreement between calculated and measured elastic angular distributions varied as the structure of the measured results changed with energy. For example, calculated and measured values were similar at 1.0 MeV, as shown in Fig. 3, but differed appreciably at 1.45 MeV, as indicated in Fig. 4. Over the full measured energy range the calculated elastic scattering generally followed the measured elastic cross sections as shown in Fig. 2.

Inelastic neutron excitation cross sections were calculated using the above "selected" spherical potential and the Hauser-Feshbach formalism.[18] The calculations explicitly considered the excitation of the 983.5 (^{48}Ti), 889.2 (^{46}Ti) and 159.6 (^{47}Ti) keV states assuming the former two are 2+ configurations and the latter a 7/2- state. The calculated cross sections for the excitation of the 2+ states tended to be slightly smaller than the experimental values as shown in Fig. 5. The calculated excitation of the 7/2- state was $\sim$ 3 mb/sr, consistent with the marginal experimental observation. Calculated inelastic angular distributions were nearly isotropic and qualitatively consistent with the measured values as illustrated in Fig. 4.

The even isotopes of titanium are deformed with two-photon (2+) vibrational first-excited states.[22] Of these the 983.5 keV state in ^{48}Ti was the major contributor to inelastic neutron processes. The excitation of these vibrational states and the effect of deformation was examined using a non-spherical optical-model with two-channel coupling.[20] The

shape-factors and the parameters of the non-spherical potential were identical to those employed in the spherical calculations, above. The nuclear deformation was varied between 0.0 and 0.3, with 0.2 being selected as consistent with the present experiments and with values reported in the literature.[20] Elastic angular distributions obtained with the deformed potential differed from those of the spherical potential and tended to give better agreement with experiment as indicated in Figs. 3 and 4. The deformed calculations also lead to improved agreement with measured inelastic cross sections as illustrated in Figs. 4 and 5. The resulting calculated inelastic angular distributions showed a small assymetry about ninety degrees (a few mb/sr) due to the direct excitation of the 2+ vibrational state. The effect was too small to be observed in the present measurements.

Calculations using the above "selected" potential were qualitatively descriptive of measured elastic angular distributions at 3.2 and 4.1 MeV[23,24] particularly when deformation was considered. Total cross sections were calculated at neutron energies to 10.0 MeV using the potential energy dependence suggested by Engelbrecht and Fiedeldey.[19] The calculated total cross sections became progressively smaller than experimental values[4] with increasing energy with an ∿ 20% difference at 10.0 MeV.

In the low energy limit the "selected" potential with either spherical or deformed calculations resulted in $\ell = 0$ strength functions (see Table 1) a factor of five or more smaller than generally found in this mass region and/or as deduced from resonance experiments.[2] This was in contrast to results obtained with potentials emphasizing strength functions rather than total cross sections and angular distributions as in the present case. For example, the potential of Moldauer (PAM),[3] defined in Table 1, well describes the mass dependence of $\ell = 0$ strength functions in this mass region. However this particular potential did not reasonably represent the

total and elastic scattering cross sections of the present work (see Figs. 1, 2, 3 and 4). The differences may, in part, be due to peculiarities in the structure of the cross sections of the titanium isotopes in the present energy range. Inelastic scattering cross sections determined from the PAM parameters and the Hauser-Feshbach formalism were appreciably larger than the measured values as shown in Fig. 5. However, Moldauer has pointed out the importance of resonance width fluctuation and correlation effects in the mass region of titanium.[25] He derived a "corrected" transmission coefficient dependent on the overlap parameter, Q, where Q varies from 1 (isolated resonances) to 0 (strongly overlapping resonances). When this correction was applied to the PAM results for the two limiting cases (Q = 0, Q = 1) a relatively good agreement between measured and calculated inelastic scattering cross sections was achieved as illustrated in Fig. 5. Thus, in the context of inelastic scattering, the choice of potential parameters was appreciably influenced by resonance width fluctuations and correlations. This influence was not as great in the area of elastic scattering cross sections.

The experimental results, particularly the total cross sections, were characterized by pronounced and partially resolved resonance structure (see Fig. 1, for example). When averaged over energy intervals of 20 to 100 keV this structure displayed a characteristic intermediate resonance behavior. This intermediate structure is evident in the elastic scattering cross sections measured with a 20 keV resolution shown in Fig. 1. Intermediate resonance structure of this type has been interpreted in terms of quasi-particle processes and of fluctuations in compound-nucleus resonance properties.[11,26,27] The intermediate resonance structure observed in the present experimental results was compared to that deduced from a statistical R-matrix formalism.[28] The cross sections calculated from the statistical R-matrix and averaged over increments equiva-

lent to those of the experiment were qualitatively similar to the measured values. Furthermore, the auto-correlation functions determined from the calculated and the measured cross sections were similar. It was concluded that the apparent intermediate structure observed in the experiment was consistent with that deduced from compound-nucleus processes by means of the statistical R-matrix. The details of this statistical interpretation are discussed elsewhere.[29]

II. Utilization of Experimental and Calculational Results in the Evaluated File

The Evaluated Nuclear Data File-B (ENDF/B)[30] contains titanium (material 1016). This evaluation was prepared by Pennington and was largely based upon prior evaluated data sets.[31] In order to make available the results of the present work and other recent experimental values in useful form and to provide for the request for basic titanium cross section data, the previous titanium ENDF file was modified and updated to include the most recent experimental values. Modifications were confined to incident energies above 0.1 MeV. Values at all lower incident energies were retained from the original file. The modification emphasized experimental values and used the model-calculations outlined above to extrapolate the measured quantities where necessary. The file requires internal consistency which is not available in detail from the experimental values primarily due to the different experimental resolutions employed in the various measurements. Thus construction of the file requires appreciable extrapolation and interpolation of measurements. Generally, the modification procedures were as follows:

A. Total Neutron Cross Sections

Total cross section values in the energy range 0.1 to 1.5 MeV were taken explicitly from the experimental results of the present work. Above an energy of 1.5 MeV experimental values from Schwartz,[32] Barschall et al.,[33] and Foster and Glasgow[34] were used. Above 10.0 MeV the measured values were extrapolated with model calculations using the potential described above normalized to experimental values at lower energies. Where necessary the measured total cross sections were linearly interpolated in energy so as to assure that the energies of the partial cross sections were a sub-set of the total cross section energies. The final evaluated total cross section is indicated in Fig. 6.

B. Elastic Neutron Scattering Cross Sections

The evaluated elastic scattering cross section was calculated directly from the evaluated total cross section and the non-elastic cross section. The non-elastic cross section was constructed from the various partial cross sections and linearly interpolated to the more detailed energies of the total cross section file. In this manner the resulting evaluated elastic cross section retained the detail of the high-resolution total cross section file and maintained internal consistency. When averaged over corresponding energy increments the evaluated elastic scattering cross sections were in good agreement with those measured in the present work. The resulting elastic evaluated file is shown in Fig. 6.

The elastic scattering angular distributions were expressed as $f_\ell(E)$ coefficients as defined by the ENDF format.[30] At neutron energies of $\leq$ 1.5 MeV these coefficients were taken explicitly from the present experimental results. Additional experimental results were used at 3.2 MeV[23] and 4.0 MeV.[24] Model-calculations, normalized to available experimental values, were used to interpolate the measurements and extrapolate the $f_\ell(E)$

coefficients to higher energies. The $f_\ell(E)$ values obtained in the above manner provide a good representation of the best available experimental information. However, they are generally based upon measurements with approximately an order of magnitude poorer resolution than that employed in total cross section studies. Thus $f_\ell(E)$ values will not display as detailed an energy dependence as either the total or elastic cross sections of the file.

C. Inelastic Neutron Scattering Cross Sections

The inelastic neutron scattering cross sections were assumed entirely due to the even isotopes of titanium (88% abundant). At incident neutron energies of $\leq$ 1.5 MeV the experimental results of the present work were explicitly used. Their components plus the cross sections due to the excitation of known states at 2.32, 2.40 and 3.2 MeV[35] were extrapolated to incident neutron energies of $\sim$ 7.0 MeV using the calculation and the potential described above normalized to the measured values. At higher energies the continuum inelastic distributions and nuclear temperatures of the original evaluation were retained. The resulting partial and total inelastic neutron scattering cross sections are shown in Fig. 7.

D. Non-Neutron Exit Channels

Radiative capture cross sections and (n:X) reaction cross sections where X $\neq$ neutron were retained from the original evaluation without modification as the present experimental results did not directly define these quantities. These non-neutron reaction cross sections were incorporated in the non-elastic cross section used to obtain the elastic file as described above. Where necessary various partial cross sections were interpolated in energy-magnitude in a linear manner.

The revised and updated ENDF file deduced in the above manner was verified using the check routine CHECKER[30] and the physical content inspected with suitable graphical procedures. The final result is an evaluated file in the widely used ENDF format fully contemporary with available microscopic cross section information and largely meeting the needs of the initial user request.

III. Tabulated Evaluated File in the ENDF/B Format

The complete revised and updated file, derived in the manner described above, is listed in the appendix.

TABLE 1: OPTICAL POTENTIAL PARAMETERS

Parameter	Potential	
	Selected	PAM
Real Well		
Depth, MeV	44.5	46.0
Radius, F	4.543	4.815
Diffuseness, F	0.62	0.62
Imaginary Well		
Depth, MeV	9.0	14.0
Radius, F	4.797	5.316
Diffuseness, F	0.50	0.50
Spin-Orbit		
Depth, MeV	7.0	7.0
Deformation Parameter[d]	0.2[a]	- -
$\ell = 0$ Strength Function X 10^4	0.52[b]	4.1
	0.74[c]	

[a]Applicable only to the deformed calculations.

[b]Spherical calculations.

[c]Deformed calculations.

[d]The direct-well was set equal to the real-well.

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FIGURE CAPTIONS

Fig. 1 Measured total and elastic scattering cross sections of titanium. The solid curve indicates the results of calculations using the "select" optical potential of Table 1 as described in the text. The dashed, PAM, curve was obtained from the potential of Ref. 3.

Fig. 2 Differential elastic scattering cross sections of titanium expressed in the format of Eq. (1). The measured values are indicated by crosses. The solid and dashed curves indicate the results of calculation based, respectively, on the spherical and deformed potentials of Table 1. The dashed-dotted curve indicates the results calculated from the potential of Ref. 3.

Fig. 3 Differential elastic scattering cross sections of titanium at 1.0 MeV. Solid data points indicate the present results, open circles those of Ref. 12 and squares those of Ref. 13.

Solid and dashed curves were obtained by calculation using the spherical and the deformed potentials of Table 1, respectively. The dashed-dotted curve was calculated from the potential of Ref. 3.

Fig. 4. Differential scattering of 1.45 MeV neutrons from titanium. Circular data points indicate measured elastic cross sections, squares inelastic cross sections. The curves were obtained by calculations as follows: 1) solid curve spherical potential of Table 1, 2) dashed curve deformed potential of Table 1, 3) dashed-dotted curve potential of Ref. 3 with no fluctuation correction, 4) dashed-dotted-dotted curve potential of Ref. 3 with fluctuation correction and overlap parameter Q = 0.0, 5) dashed-dotted-dotted-dotted as per 4) but with Q = 1.0.

Fig. 5 Cross sections for the inelastic neutron excitation of 889.2 and 983.5 keV states in titanium. Crosses indicate results of fine resolution measurements, boxes broad resolution results. Curves indicate the results of calculation as follows: 1) solid curve; spherical potential of Table 1, 2) dashed curve deformed potential of Table 1, 3) dashed-dotted curve; the potential of Ref. 3 with no fluctuation correction, 4) dashed-dotted-dotted curve as per 3) but with fluctuation correction and overlap parameter Q = 0.5.

Fig. 6 Evaluated total and elastic-scattering cross sections of titanium, 0.1 to 18.0 MeV.

Fig. 7 Evaluated inelastic-scattering, (n,γ), (n,p), $(n,2n)$ and (n,α) cross sections of titanium; 0.01 to 18.0 MeV.

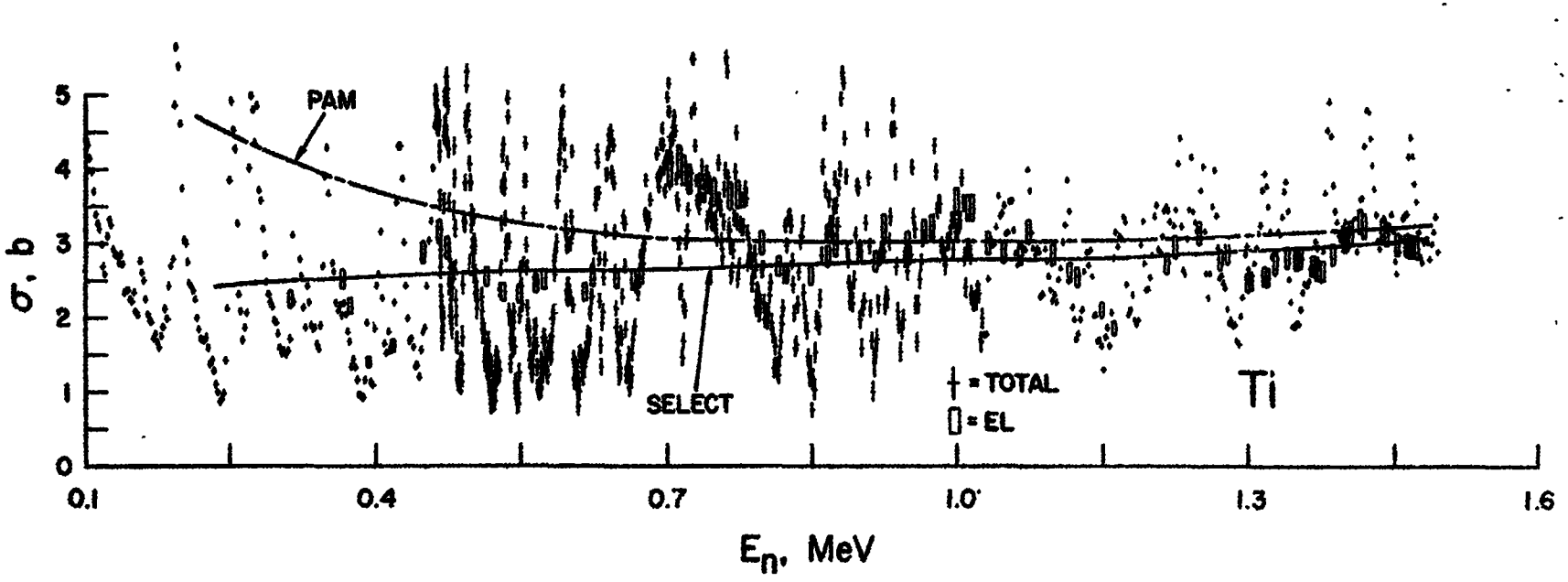

Figure 1.

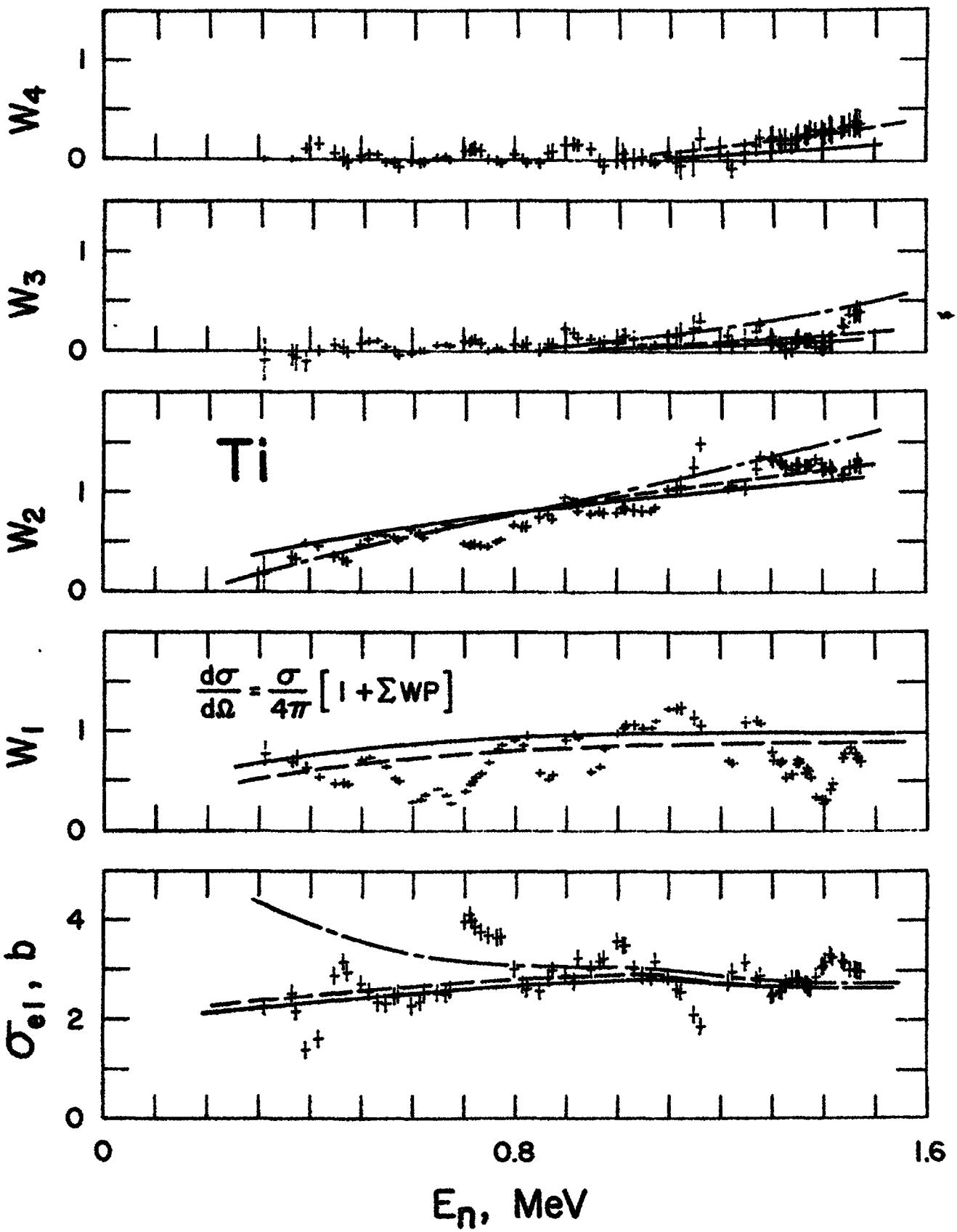

Figure 2.

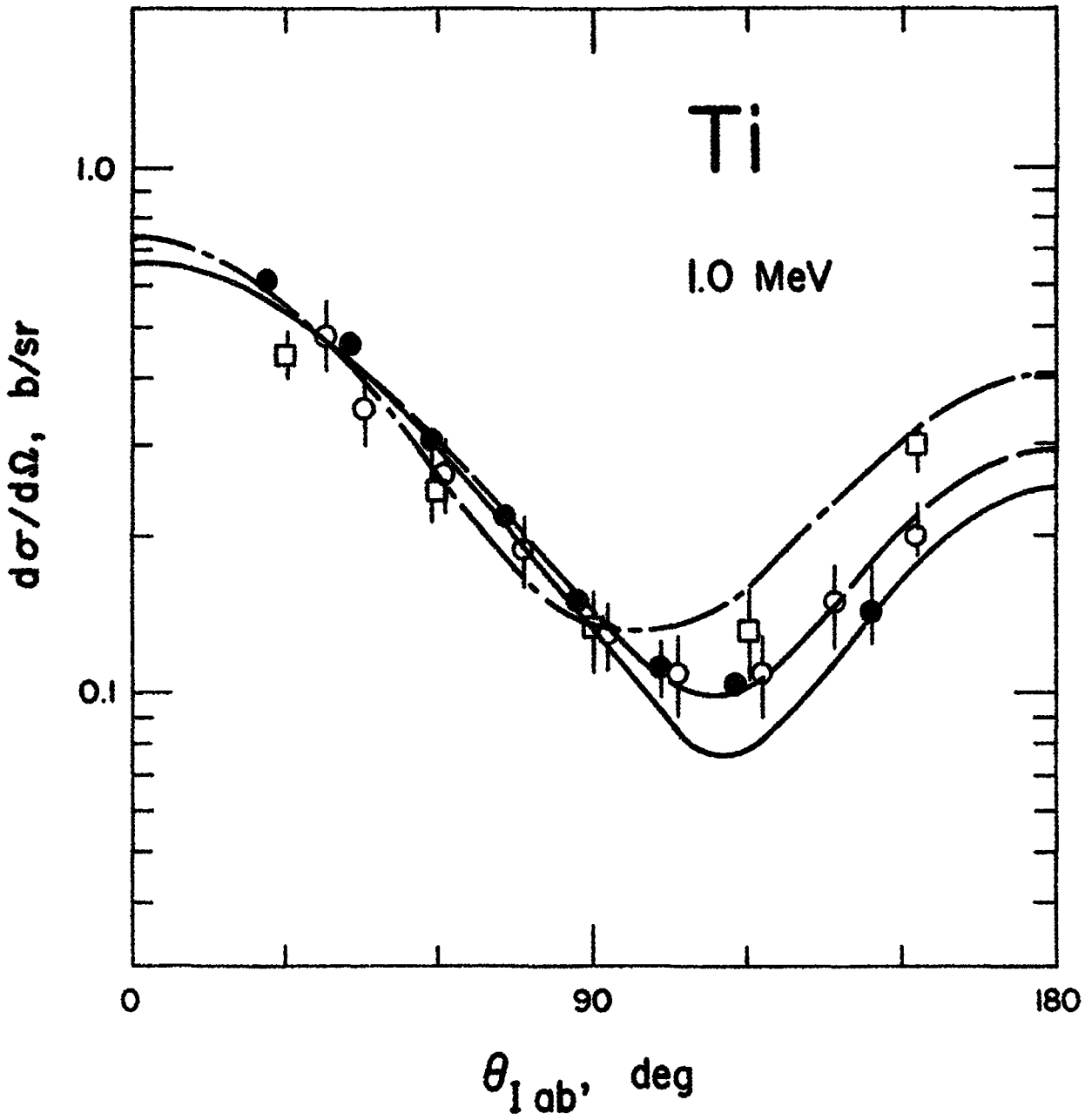

Figure 3.

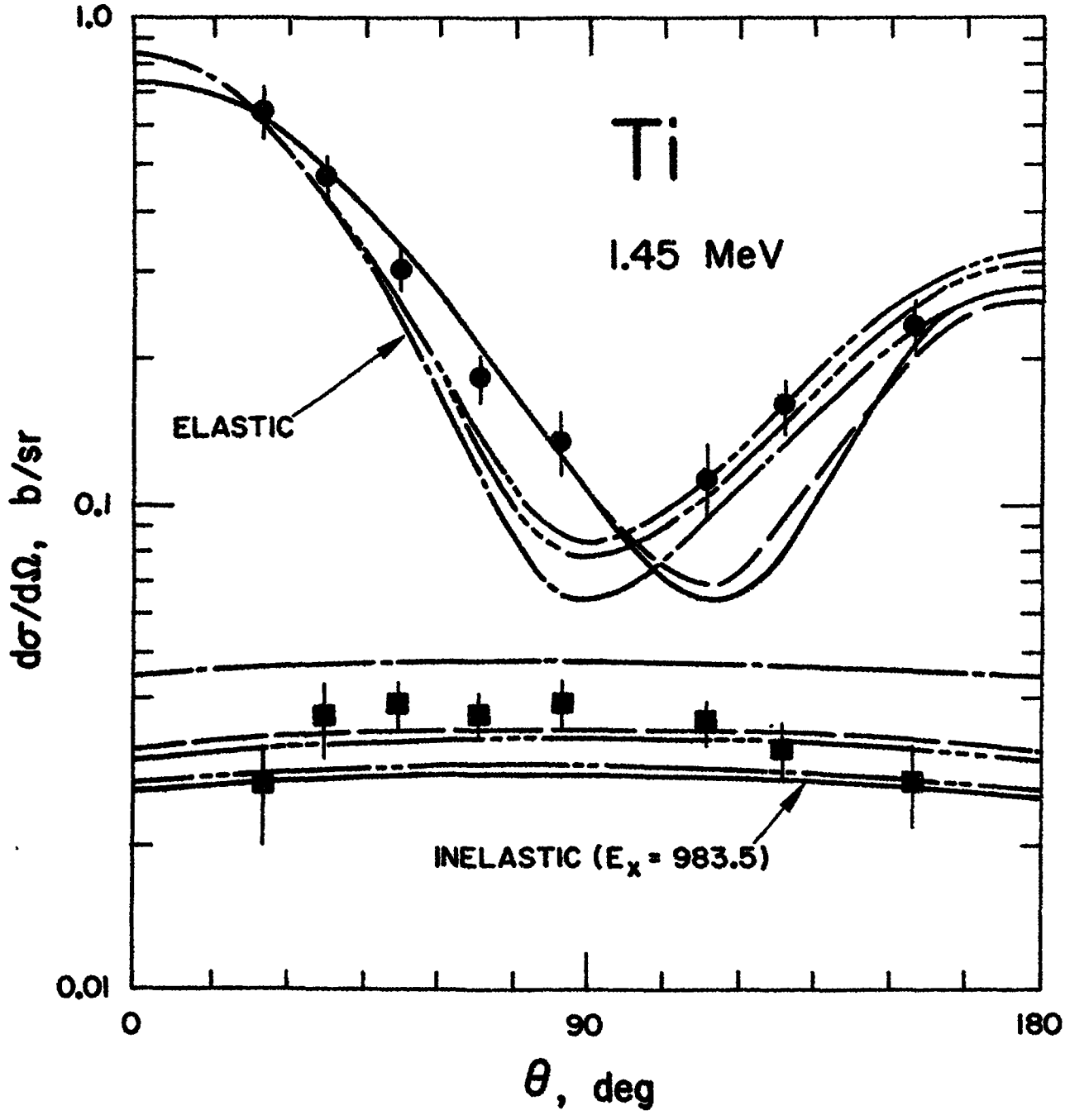
1.0
0.1
0.01
Ti
1.45 MeV
ELASTIC
INELASTIC (E_x = 983.5)
dσ/dΩ, b/sr
0
90
180
θ, deg

Figure 4.

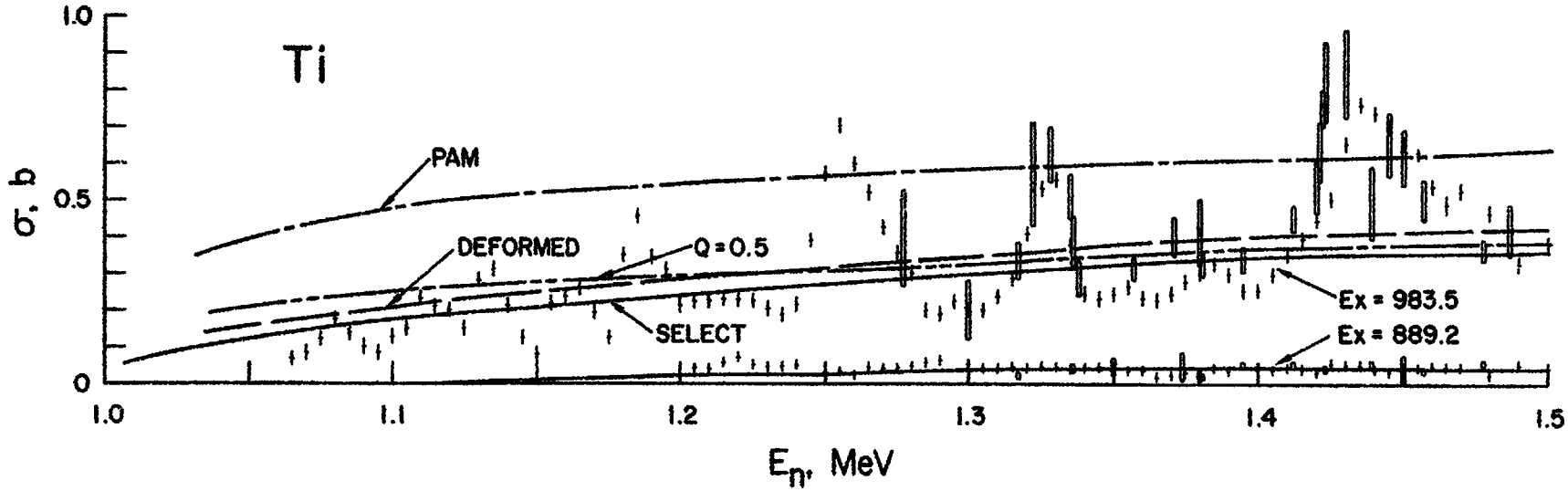
Ti
PAM
DEFORMED
Q = 0.5
SELECT
Ex = 983.5
Ex = 889.2
σ, b
1.0
0.5
0
1.0
1.1
1.2
1.3
1.4
1.5
E_n, MeV

Figure 5.

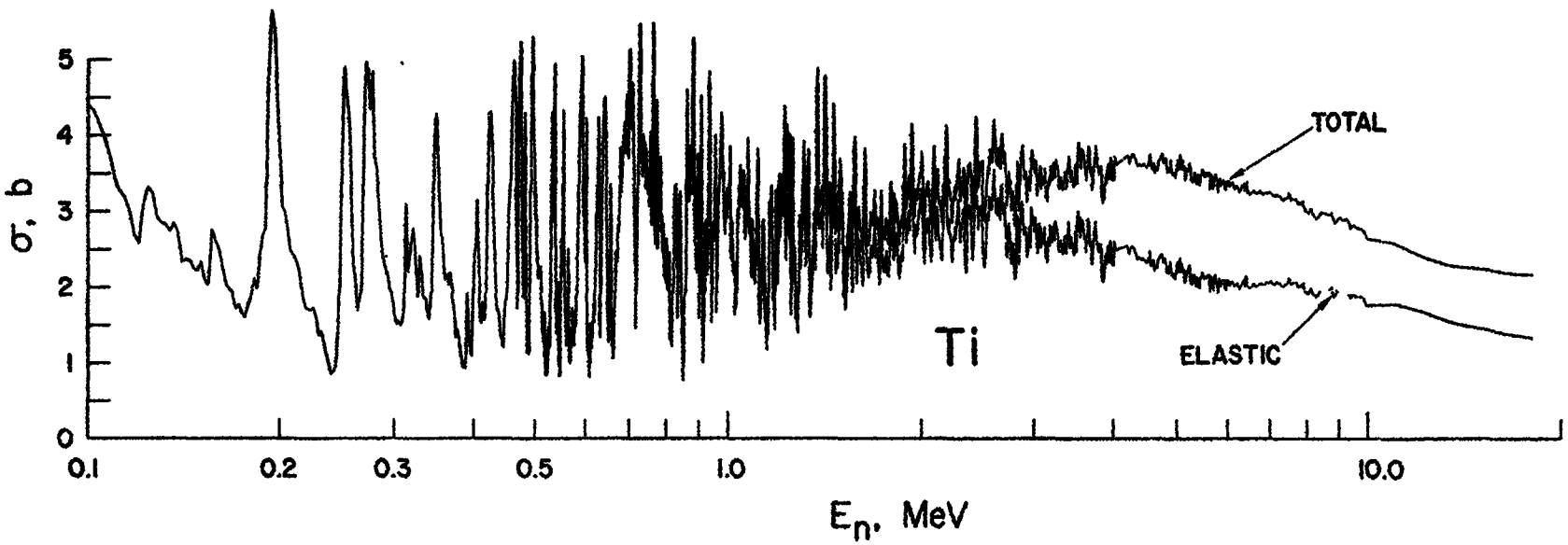

Figure 6.

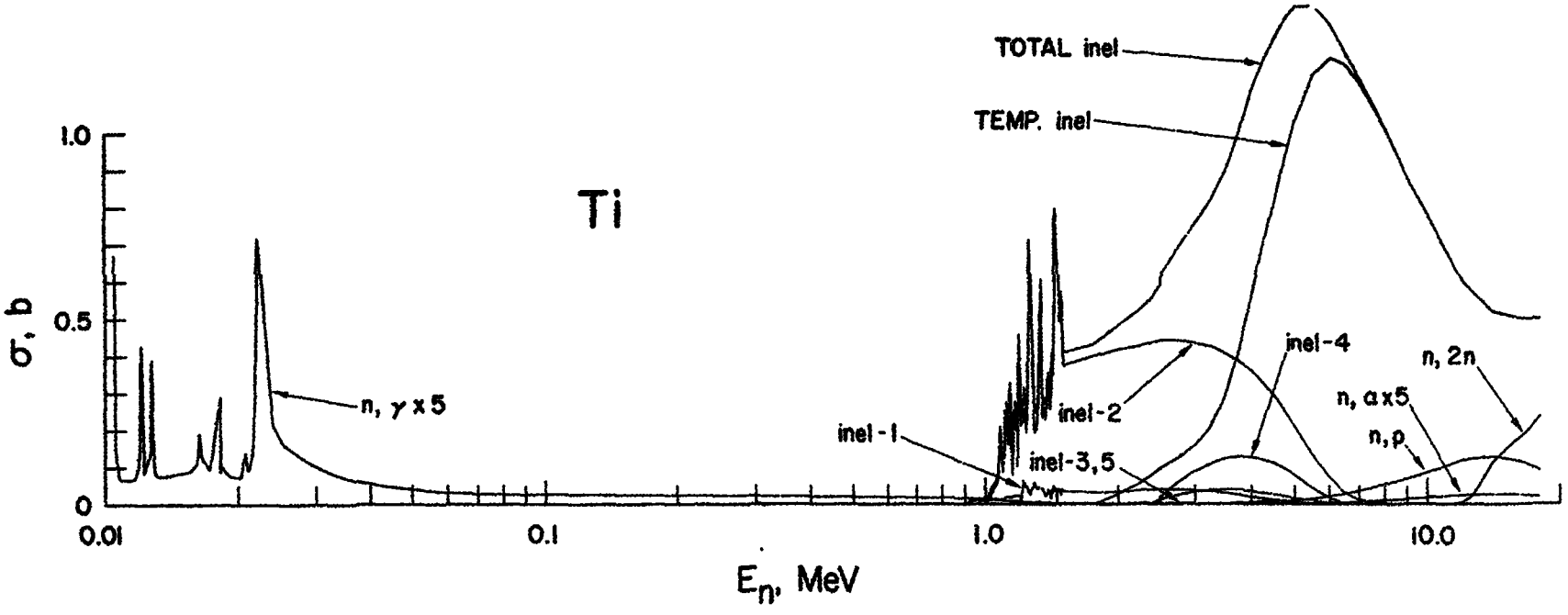
Ti
TOTAL inel
TEMP. inel
inel-4
n, 2n
inel-2
n, α x5
n, p
inel-1
inel-3,5
n, γ x5
σ, b
1.0
0.5
0
0.01
0.1
1.0
10.0
E_n, MeV

Figure 7.

Appendix:

Note: The complete revised and tabulated evaluated file for Titanium in the ENDF/B format has not been reproduced in this Appendix but is available, on request, from the IAEA Nuclear Data Section.

Fast Neutron Cross Sections of ^{240}Pu; Measured Results and a Comparison with an Evaluated File

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Abstract

Fast neutron total cross sections and elastic- and inelastic-scattering cross sections of ^{240}Pu are reported. The total cross sections are measured from neutron energies of 0.1 to 1.5 MeV in increments of $\sim$ 25 keV. The elastic-scattering cross sections are measured at $\lesssim$ 50 keV intervals from incident neutron energies of 0.3 to 1.5 MeV. The inelastic neutron excitation cross sections of states at 42 $\pm$ 5, 140 $\pm$ 10, 300 $\pm$ 20, 600 $\pm$ 20 and 900 $\pm$ 50 keV are measured. The experimental results are discussed in the context of the optical, compound-nucleus and direct-reaction nuclear models including the effects of resonance width fluctuations and the fission process. The measured results are critically compared with the corresponding quantities in the evaluated nuclear data file ENDF/B.

I. INTRODUCTORY REMARK

The isotope ^{240}Pu is a major constituent of many fast-breeding reactors wherein the plutonium fuel may consist of $\lesssim$ 20 percent ^{240}Pu.[1] Therefore fast neutron interactions with this isotope are a consideration in the neutronic design of these systems. Despite this applied importance the experimental microscopic fast neutron cross sections of ^{240}Pu are relatively unknown and a number of requests for measured information are outstanding.[2] Major reliance continues to be placed upon evaluated data sets based largely on nuclear-model estimates.

The fission neutron cross section of ^{240}Pu has been reasonably well measured.[3,4,5] It is large with a relatively low energy threshold. At low energies the fission cross section is of interest in the context of fission theory due to its sub-threshold characteristics.[6] Experimental total cross sections and elastic- and inelastic-scattering cross sections of ^{240}Pu above $\sim$ 100 keV are experimentally essentially unknown. This ignorance is, in part, due to the limited availability of suitable samples and to experimental problems associated with the high spontaneous fission rate of the material.[7] The present work was undertaken in an effort to generally improve experimental understanding of the fast neutron cross sections of ^{240}Pu by direct measurement of total and of scattering cross sections to $\sim$ 1.5 MeV and to specifically satisfy requests for fast neutron ^{240}Pu data. It was also the objective to; provide a reasonable experimental foundation for the nuclear models employed in the interpolation and extrapolation of measured quantities, and to obtain additional insight into nuclear structure and fission properties in the trans-uranium region.

II. EXPERIMENTAL METHODS

The experimental measurements were made possible through the availability of a 54 gm sample of plutonium $\sim$ 100% enriched in the isotope ^{240}Pu. The material was a metal foil 98.7 weight-percent plutonium and 1.3 weight-percent aluminum. It was formed into a cylindrical sample 2.0 cm in diameter by pressing the foil into a 0.013 cm thick stainless steel can. The uniformity of the sample density was governed by the pressing procedure. The sample was, in itself, an appreciable fast neutron source due to spontaneous fission.

Total neutron cross sections were deduced from the observed transmission of essentially mono-energetic neutrons through the ^{240}Pu sample

assuming a uniform sample density. The measurements were made at ∿ 5 keV intervals with ∿ 5 keV resolution from incident neutron energies of 0.1 to 1.5 MeV. Sample transmissions were ∿ 75%. The statistical precision of the measured cross sections was ∿ 1%. Small corrections were made for "in-scattering" and background contributions and the fidelity of the apparatus verified by determination of the well known total neutron cross sections of carbon.[3,8]

The neutron scattering cross sections were measured using the pulsed-beam fast time-of-flight technique. The apparatus consisted of collimated detectors which concurrently measured neutrons scattered at eight laboratory angles. The $^{7}Li(p,n)^{7}Be$ neutron source was so arranged as to provide an incident neutron resolution at the scattering sample of ∿ 20 keV. The scattered neutron velocity resolution was generally ∿ 1.5 nsec/M. All scattering cross sections were determined relative to the known differential elastic scattering cross sections of carbon[9] and corrected for multiple-scattering and other experimental perturbations.

The specific details of the total and scattering apparatuses and methods are described elsewhere.[10,11]

III. EXPERIMENTAL RESULTS[a]

A. Total-Neutron Cross Sections

The measured total cross sections displayed considerable energy-dependent structure which was well correlated with known prominent resonances in the total cross section of aluminum. The primary results were corrected for the 1.3 weight-percent aluminum content of the sample using

[a]A numerical tabulation of all measured values is given in the Appendix and all experimental results have been transmitted to the National Neutron Cross Section Center, Brookhaven National Laboratory.

aluminum total cross sections measured at this Laboratory[12] and smoothed by averaging the corrected values over 25 keV intervals. The final corrected and averaged results are shown in Fig. 1. The remaining structure near 530 keV is believed a residual artifact due to uncertain corrections for the effects of the large aluminum resonance in this region and to have no physical significance. The errors associated with the results were largely of a systematic nature and, particularly, are due to the uncertain transmission-density of the sample. The combined total-cross-section error was conservatively estimated at five percent and the mean deviation of the measured values for a smooth curve was generally appreciably less.

No previously reported total cross sections of ^{240}Pu in the energy range of the present experiments were found in the literature. The measured partial elastic- and inelastic-scattering cross sections (see below) were combined with the reported fission cross section[3] for comparison with the directly measured total cross sections. As shown in Fig. 1, the agreement was good with no discrepancy greater than $\sim$ 300 mb. This consistency indicates that both total and partial cross sections have been reasonably determined.

B. Elastic-Neutron-Scattering Cross Sections

The differential elastic-scattering cross sections were deduced from the measured time-of-flight (TOF) spectra with careful attention to background effects. Each TOF distribution was corrected for non-sample associated backgrounds inclusive of contributions due to the sample container using direct experimental measurements. After this correction there remained an appreciable fission-neutron background, time-uncorrelated from ^{240}Pu spontaneous fission and time-correlated from neutron-induced fission. Both fission-neutron backgrounds were estimated using a least-square fitting procedure. Time intervals were selected from each TOF distribution in such

a manner that elastic- and/or inelastic-scattered neutrons were either physically inadmissable (for example, at times before detection of the elastic event) or were judged to make no significant contribution to the selected interval. The measured data in these selected time intervals was fitted with a low-order power series in time (usually quartic) which reasonably interpolated the fission-neutron background over the entire TOF distribution. The fission-neutron contribution determined from the fitting procedure was subtracted from the measured TOF spectra.

The ^{240}Pu elastic-scattering component was obtained in such a manner as to include neutrons elastically-scattered from the aluminum contaminant of the sample. At forward scattering angles ($\sim$ 30 deg.) the aluminum contribution was indistinguishable from the primary ^{240}Pu elastic events. At backward scattering angles ($\sim$ 155 deg.) and, particularly, at higher energies the two elastic components were well separated due to the different energy transfer to the recoiling nucleus. In these instances considerable attention was given to the correct evaluation of the aluminum elastic contribution in the presence of inelastic neutrons resulting from the excitation of the 42 and 140 keV states in ^{240}Pu.

The combined ^{240}Pu and aluminum differential elastic scattering cross sections were determined from incident energies of 0.3 to 1.5 MeV in increments of $\lesssim$ 50 keV and at eight scattering angles between $\sim$ 25 and $\sim$ 155 degrees. The measurement angles varied slightly from distribution to distribution but were typically 28, 38, 53, 68, 84, 114, 128 and 154 degrees. The resulting differential cross sections were least-square fitted with the expression

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi} \left(1 + \sum_{i=1}^{5} \omega_i P_i\right) \qquad (1)$$

where σ (angle-integrated cross section) and ω_i coefficients were determined from the fitting procedure and P_i are Legendre polynomials expressed

in the laboratory system. The differential elastic-scattering cross sections, expressed in the form of Eq. (1), were corrected for the aluminum contamination using the aluminum elastic-scattering cross sections of Ref. 13. The scattered neutron resolution was not generally sufficient at incident energies of $\gtrsim$ 1.0 MeV to differentiate the elastic neutron group from inelastic neutrons resulting from the excitation of the 42 keV state in ^{240}Pu. Careful measurements at selected angles with an improved resolution of $\sim$ 0.75 nsec/M qualitatively established the inelastic component to $\sim$ 1.3 MeV. Assuming an isotropic inelastic neutron distribution and interpolating and extrapolating measured inelastic values with theoretical guidance (see below), the measured elastic cross sections were corrected for inelastic neutron contributions above $\sim$ 1.0 MeV. This correction was small at forward scattering angles but appreciable at large scattering angles. However, uncertainties in the inelastic correction procedure did not significantly contribute to errors in the angle-integrated elastic scattering cross section values.

The fully corrected results were well described by Eq. (1) throughout the measured angular interval. However, extrapolation of the measurements beyond this interval, particularly to backward angles, may not be reliable and may even lead to illicit cross sections. Uncertain behavior of Eq. (1) beyond the measured interval did not appreciably effect the deduced angle-integrated cross sections nor were they significantly influenced by alternate termination of the series of Eq. (1) at i = 4 or 5.

Representative differential elastic-neutron-scattering angular distributions are shown in Figs. 2A and 2B. Due to the complexities of the correction procedures, outlined above, the uncertainties associated with the measured differential cross sections were based on subjective judgements. It was estimated that the error in the measured differential values varied from 5-10% at forward angles to as much as 30-50% at extreme back-

ward scattering angles. These uncertainty estimates included errors associated with the carbon reference standard. The behavior of the elastic scattering results over the entire measured energy range is summarized in Fig. 3 in the format of Eq. (1). The uncertainties associated with the angle-integrated elastic cross sections were estimated to be 8-10% and the illustrated uncertainties in the omega coefficients are indicative of the quality of the fit of Eq. (1) to the measured data.

Elastic-scattering cross sections of ^{240}Pu have apparently not been previously measured at the energies of the present experiments. However, the present elastic-scattering results are reasonably consistent with the measured total and inelastic-scattering neutron cross sections as discussed above.

C. Inelastic-Neutron-Scattering Cross Sections

The differential inelastic-neutron-scattering cross sections were determined from the respective neutron groups observed in the TOF spectra. The background and other experimental-correction procedures were generally carried out as outlined above in the context of elastic scattering. Inelastic measurements were made concurrently with elastic-scattering determinations. However, at some incident energies and scattering angles the experimental results associated with the excitation of low energy excited states were rejected because of undue contributions from neutrons elastically scattered from the aluminum contaminant of the ^{240}Pu sample. This contaminant effect was most troublesome at incident energies $\gtrsim$ 700 keV with the consequent increased uncertainty in the measured values in the higher energy region. The second neutron group from the ^{7}Li(p,n)^{7}Be source reaction, elastically scattered from the sample, distorted inelastically scattered neutron components corresponding to reaction Q-values of $\sim$ -500 keV. No prominent inelastic component was experimentally observed in this region

but a small contribution would have been so masked as to escape notice. Where reasonably defined the observed inelastic angular distributions were essentially isotropic. Thus the angle-integrated inelastic neutron excitation cross sections were obtained from a simple average of the measured differential values multiplied by 4π. Throughout the work the experimental emphasis was on inelastic cross section magnitudes for applied use rather than on nuclear structure information often better obtained by other means.

Inelastic-neutron-excitation cross sections corresponding to states at 42 ± 5, 140 ± 10, 300 ± 20, 600 ± 20 and 900 ± 50 keV were observed. Further, neutrons corresponding to the excitation of states at energies $\gtrsim$ 1.0 MeV were qualitatively observed but subject to large background effects which made quantitative interpretation unreliable and therefore the respective cross sections are not reported here. The excitation energies were determined from the neutron flight-times and verified by observation of well known inelastic-neutron processes (for example, ^{56}Fe Q = -850 keV).[14] The energy uncertainties associated with the various neutron groups reflect estimates of experimental accuracy and the apparent contribution to some of the inelastic groups of several components. The observed structure is summarized and correlated with more detailed information reported in the literature in Fig. 4.[7]

The above excitation cross sections associated with the above neutron groups are outlined in Fig. 4. The indicated uncertainties are based upon estimates inclusive of experimental errors and those associated with the carbon reference standard. No comparable microscopic cross sections have, apparently, been previously reported. However, the magnitudes of the measured inelastic cross sections are consistent with the total and elastic-scattering cross section results described above.

IV. CALCULATION AND DISCUSSION

The interpretation of the experimental results was primarily based upon optical- and statistical-nuclear models.[15,16] The point of departure was an optical potential of the form

$$V(r) = - Vf(r) - iWg(r) - V_{so}h(r)\ \underline{\ell}\cdot\underline{\sigma}, \qquad (2)$$

where f(r) was of the Saxon form, g(r) a guassian surface form, and h(r) a Thomas form.[15] Over the energy range of the present experiments the potential parameters were assumed energy-independent. Compound-nucleus processes were calculated using the Hauser-Feshbach[16] formula with fluctuation corrections

$$\overline{\sigma}_{cc'} = \pi\lambda^2 \frac{T_c T_{c'}}{\sum_{c'',T_{c''}} T_{c''}} \cdot F_{cc'} \qquad (3)$$

where T_c are conventional transmission coefficients and $F_{cc'}$ the resonance-width-fluctuation correction.[17] Fission was considered but radiative capture was assumed small and ignored. ^{240}Pu is known to be appreciably deformed and thus the basic spherical potential of Eq. (2) was extended to include the effects of collective deformation.[18,19,20]

The fission cross section of ^{240}Pu rises from low sub-threshold values, through a threshold at 600 - 800 keV to large values of ∿ 1.5 b at ∿ 1.0 MeV and above.[3] Compound-nucleus decay through fission will be prominent over much of the energy range of the present experiments. The initial objective was the determination of a neutron model descriptive of total neutron cross sections throughout the measured interval and of partial reaction cross sections below ∿ 600 keV where fission contributions were small. Using this neutron model attention was given to partial reaction cross sections, including fission, at incident energies above ∿ 600 keV. Parameters suitable for the description of fast neutron processes in the similar nucleus ^{238}U were taken as the starting point with adjustments to achieve

a "good" description of measured values.[21] The selected spherical potential parameters are summarized in Table 1. Deformation was introduced for values of the parameter $\beta \leq 0.3$ using the spherical potential in a rotational coupled-channel model.[20]

Calculated total-neutron cross sections are compared with the corresponding measured values in Fig. 1. The spherical ($\beta = 0.0$) results agree with or are slightly smaller ($\lesssim$ 250 mb) than the measured values. The calculated values increase with β, becoming as much as 600 mb larger than the experimental values for $\beta = 0.3$. The β of ^{240}Pu reported from studies of other nuclear processes is in the range 0.2 to 0.3 [18] and generally resulted in calculated total cross sections appreciably larger than the experimental values.

Calculated and measured differential elastic-scattering angular distributions at 400 keV are compared in Fig. 2A. Both spherical and deformed calculated results are inclusive of compound-nucleus contributions with fluctuation and overlap corrections. The latter were determined using Moldauer's transmission coefficients, θ_α, with overlap parameter $Q = 0.5$ as defined in Eq. (4).[17]

$$\theta_\alpha = T_\alpha + \frac{1}{Q_\alpha}\left[1 - (1 - Q_\alpha T_\alpha)^{\frac{1}{2}}\right]^2 \qquad (4)$$

Where T_α is the transmission coefficient of Eq. (3).

The results were not strongly dependent on the choice of Q and its selection was primarily governed by fission considerations (see below). The calculated and measured distributions of Fig. 2A are in qualitative agreement, with discrepancies of the same magnitude as those resulting from changes of $\Delta\beta$ by $\sim$ 0.1. These comparisons tended to indicate a β of $\sim$ 0.2.

Measured and calculated inelastic excitations of the 42 keV (2+) state below $\sim$ 600 keV were in qualitative agreement as illustrated in

Fig. 4. At these lower energies the calculated cross section increased with deformation primarily due to larger calculated reaction cross sections with little contribution ($\lesssim$ 100 mb) from direct processes. Concurrently, large deformation generally led to calculated total cross sections appreciably larger than the experimental values as is evident in Fig. 1. The omission of the fluctuation and overlap effects led to calculated values rather higher than indicated by experiment.

Calculated $\ell = 0$ strength functions determined with both spherical ($\beta = 0.0$) and deformed ($\beta = 0.1, 0.3$) potentials are outlined in Table 1. Comparable values deduced from resonance measurements and systematics[22,23] are reported in the range $\sim 1\text{-}2 \times 10^{-4}$, again indicating $\beta \sim 0.2$.

It was concluded that the above neutron model, summarized in Table 1, was a suitable basis for subsequent calculations at higher energies where the fission process is pronounced.

Fission was introduced by means of transmission coefficients (see Eq. (3)) and the respective cross sections calculated using the computer program NEARREX.[19] The fission transmission coefficients, T_f, were assumed to rise to a value close to unity above the fission threshold and the overlap parameter Q was adjusted to obtain agreement between calculated and measured fission cross sections.[3] Concurrently, agreement with the observed inelastic excitation of the 42 keV (2+) state was sought. The latter objective was restrictive as choices of T_f and Q describing fission often led to smaller excitations of the 42 keV state than observed experimentally. Generally, the best low-energy ($\lesssim$ 700 keV) agreement with experiment was obtained assuming fission was predominently in the $J = 1/2+$ channel. However, even when saturated, this channel did not account for the large fission cross sections above threshold. Thus additional $J = 1/2-$ and $3/2-$ fission channels were introduced at an incident energy of $\sim$ 600 keV. With these additional fission channels calculated fission cross sections were

similar to the experimental values. Interestingly, the measured ^{240}Pu fission cross section shows structure near 600 keV, the energy where the model introduces additional fission channels. The selection of fission transmission coefficients was sensitive to the choice of the overlap parameter, Q, with Q = 0.5 giving the best overall agreement with experiment. The fission model outlined above is not inconsistent with either the double barrier concept of fission[6] or the results of experimental studies of resonance structure in sub-threshold fission[25] both of which suggest a J = 1/2+ fission channel at low energies.

Calculated inelastic excitation cross sections corrected for fission, fluctuation and overlap effects, were in reasonable agreement with the measured values as illustrated in Fig. 4. The excitation of the 42 keV state calculated using the spherical potential was marginally lower than the experimental values over the entire energy range. The deformed potential with channel-coupling and $\beta = 0.2$ or 0.3 gave results very similar to the experimental values. At higher energies ($\gtrsim$ 1.0 MeV) the direct process makes a significant contribution to the inelastic cross section ($\sim$ 200 mb) with resulting cross sections higher than those obtained without deformation. The somewhat better agreement between measured and calculated inelastic excitations of the 42 keV state obtained with larger β's was not without detrimental consequences in the area of total cross sections (see Fig. 1). The excitation of energy states above 42 keV inclusive of states to $\sim$ 1.5 MeV was calculated only with the spherical potential using spin and parity assignments of Ref. 7 as shown in Fig. 4. In these cases the agreement with experiment was good particularly in view of the available experimental resolution and of uncertainties in the excited structure that has been reported for ^{240}Pu or as can be deduced from the present measurements. There was no experimental evidence for the state reported at $\sim$ 740

keV. This was not surprising as, with the reported spin of this state, the calculated cross sections were small.

Calculated and measured angle-integrated elastic-scattering cross sections were similar (see Fig. 1) with discrepancies within the range of reasonable uncertainties in β, and experimental values. Calculated elastic-scattering angular distributions at energies above ∿ 1.0 MeV were less satisfactory as illustrated in Fig. 2B. The difference between calculation and experiment was particularly evident in the Legendre format of Eq. (1) (see Fig. 3). The discrepancies are larger at backward scattering angles and for small deformations. At energies $\gtrsim$ 1.0 MeV the calculated distributions consist essentially of shape-elastic scattering. For small β values the shape-elastic distribution has low minimia not experimentally observed. For larger β (∿ 0.2-0.3) the calculated results at backward angles were more similar to the experimental quantities but the forward angle values tended to be too large. A compromise choice of β ∿ 0.2 seemed most desirable in the context of the elastic-angular distributions.

The calculations assumed a constant overlap parameter, Q, for all channels. Perhaps more desirable would be a large Q in the fission channels with smaller values in neutron channels. The option of variable Q was not available in the computational framework. Very likely improved agreement with experiment could be obtained by detailed adjustments of the potential parameters using a specifically selected β value. Generally it was felt that the Q uncertainty, experimental uncertainties, possible alternative β values and uncertainties in fission-transmission coefficients were such that a more detailed potential parameter adjustment to possibly achieve a better description of the experimental results was not warranted.

The above procedures, while having physical merit, are costly and complex and involve the selection of a number of uncertain parameters.

From a pragmatic point of view a simpler statistical adjustment of partial reaction cross sections to account for known fission cross sections, as described in Ref. 21, can give essentially the same numerical results as obtained above. The simpler calculation may be more convenient for providing numerical values for applied purposes.

V. COMPARISON WITH THE ENDF/B EVALUATED FILE

The results of the above experiments are quantitatively compared with the relevant contents of the ENDF/B evaluated file.[25]

The measured and evaluated total-neutron cross sections are in reasonable agreement over the entire experimental energy range as illustrated in Fig. 5. The discrepancies near 500 keV are not judged significant as they could be attributed to experimental errors as discussed in Sec. III, above. At energies above 1.0 MeV the evaluated results tend to be systematically larger than the measured values but the difference is small, less than 300 mb.

Measured and evaluated elastic-scattering cross sections differ from one another in both shape and magnitude as shown in Fig. 5. The evaluated quantities are slightly larger than the measured values near 500 keV and pronouncedly lower at 1.0 MeV and above. At the higher energies the discrepancies are a full barn.

Evaluated cross sections are given for the excitation of states at 43, 142, 296, 599, 863, 903 and 945 keV. These energies are very similar to those measured in the present experiments with the latter three being experimentally observed as a composite state with an average excitation energy of 900 keV. The evaluated and measured inelastic-excitation cross sections are compared in Fig. 6. Below 500 keV the evaluated results for the excitation of the 42 keV state are in agreement with experimental observation. However, at higher energies the evaluated results are much

larger than either the corresponding experimental values or those deduced from the model discussed in Sec. IV, above. Moreover, the energy dependent shape of the evaluated cross section is not consistent with measurement or microscopic calculation. This is puzzling. As discussed in Sec. IV, the competition from fission will appreciably reduce this cross section above the fission threshold and lead to a characteristic shape of the excitation function near the fission threshold. The shape is qualitatively evident from even simple-model considerations. The evaluated and measured cross sections for the excitation of the 140 keV state are similar. The agreement is not so good for the excitation of the 300 keV state but the cross sections are small and as a consequence experimentally uncertain and of minor importance in the context of applied use. The agreement between measured and evaluated cross sections for the excitation of the 600 keV state is fairly good with the evaluated result tending to be somewhat lower. The combined evaluated cross sections for the excitation of the 863, 903 and 945 keV should be compared with the single observed composite state at an average energy of 900 keV. These combined results are about twice as large as the experimental values. This is difficult to explain unless the spin and parity assignments used in deducing the evaluated quantities differed appreciably from those used here and defined in Fig. 4 or the measured values are in appreciable error. Alternate choices of spin and parity can be questioned in the context of other experimental evidence.

Generally, it is concluded that the evaluated file is reasonably descriptive of the measured total-neutron cross sections. In the areas of elastic- and inelastic-scattering cross sections there are appreciable discrepancies between the measured and evaluated results. These will, of course, be reflected in discrepancies in associated quantities such as the non-elastic cross section as internal consistency of the file is manditory.

It is suggested that the observed discrepancies may be due to inappropriate consideration of the fission process in the calculations from which the file was largely deduced.

VI. CONCLUSION

The experimental results reasonably defined total and elastic- and inelastic-scattering neutron cross sections of ^{240}Pu over a region of previous uncertainty. The experimental results directly pertained to requests for nuclear data and suggested some revision in widely used evaluated cross sections particularly in the area of neutron scattering. A neutron-optical model was proposed based largely upon measured total-neutron cross sections and partial-neutron cross sections below the fission threshold energy of $\sim$ 600 keV. The model was inclusive of fluctuation and overlap corrections and of nuclear deformation. The model was extended to include major contributions from the fission process near and above the threshold. Comparison of calculated and measured fission cross sections and inelastic excitations of the 42 keV (2+) state suggest that fission near and below threshold is predominently in the J = 1/2+ channel with additional fission-channels opening as the incident neutron energy passes across the fission threshold. When inclusive of fission processes the model was reasonably descriptive of total and angle-integrated elastic- and inelastic-scattering experimental cross sections throughout the measured energy range and provided a suitable framework for interpolation and extrapolation. The model was less successful in the area of differential elastic cross sections at energies $\gtrsim$ 1.0 MeV.

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TABLE 1: OPTICAL MODEL POTENTIAL PARAMETERS

V	(real depth), MeV	41.5
R_1	(real radius), F	8.20
a	(real diffuseness), F	0.47
W	(imaginary depth), MeV	6.14
R_2	(imaginary radius), F	8.20
b	(imaginary width), F	1.00
V_{so}	(spin-orbit depth), MeV	7.5
Q	(overlap parameter)	0.5
β	(deformation parameter)[a]	
	case a, (spherical)	0.0
	case b,	0.1
	case c,	0.3
S_o	(ℓ = 0 strength function) x 10^4	
	case a, (spherical)	0.73
	case b,	0.91
	case c,	2.37

[a]Direct well assumed equal to real well.

FIGURE CAPTIONS

Fig. 1 Measured total (crosses) and elastic-scattering (boxes) neutron cross sections of ^{240}Pu. Solid curve indicates the total-scattering cross section deduced from the present measurements. Dashed curves show results of model calculation as discussed in Sec. IV of the text.

Fig. 2 Measured and calculated differential elastic scattering cross sections of ^{240}Pu at 400 (A) and 1200 (B) keV. Curves indicate calculated results as described in Sec. IV of the text. Data points are measured at or near the stated neutron energies.

Fig. 3 Differential elastic scattering cross sections of ^{240}Pu expressed in the format of Eq. (1). Crosses are results deduced from measured values. Curves are derived from calculations (see Sec. IV of the text).

Fig. 4 Inelastic neutron excitation cross sections of ^{240}Pu. Crosses indicate measured cross sections and associated errors for the individual excited states. Curves result from calculation as described in Sec. IV of the text. The insert correlates the reported excited structure of ^{240}Pu[7] with that observed in the present measurements (boxes). The energy dimensions of the boxes indicate the effective experimental resolutions and the brackets associate the experimental results with reported structure.

Fig. 5 A comparison of measured total- (crosses) and elastic-scattering (boxes) cross sections with comparable quantities from the ENDF evaluated file (curves).[25]

Fig. 6 A comparison of measured inelastic neutron excitation cross sections (crosses) with the respective quantities of the ENDF file (curves)[25]

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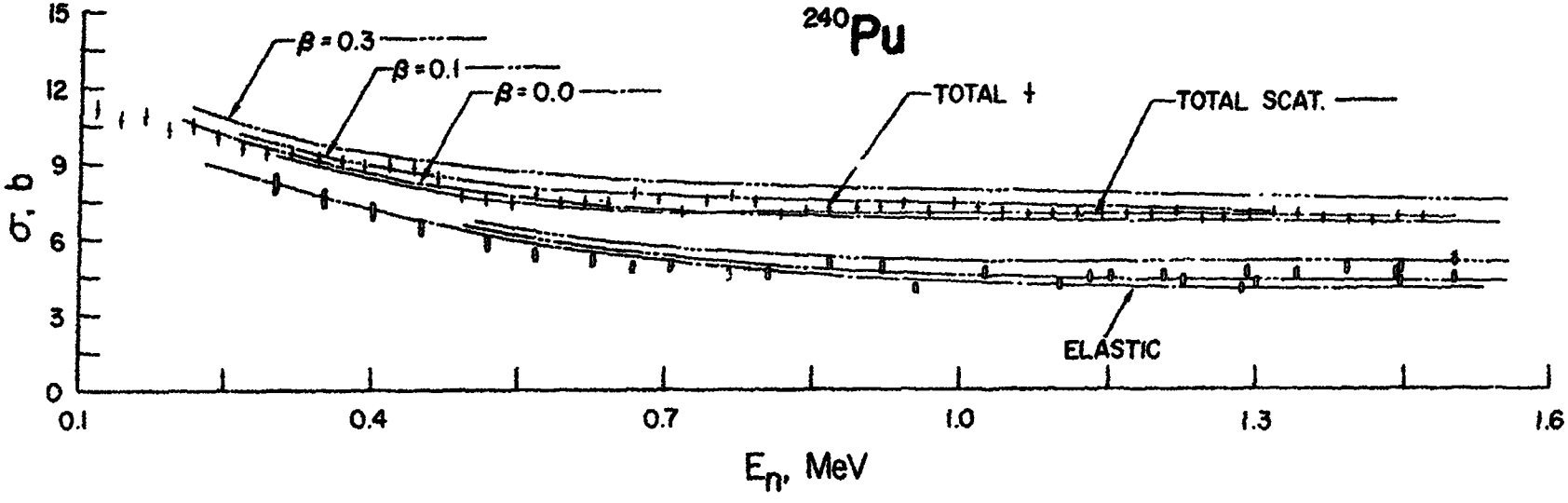
240Pu
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β = 0.1
β = 0.0
TOTAL †
TOTAL SCAT.
ELASTIC
σ, b
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12
9
6
3
0
0.1
0.4
0.7
1.0
1.3
1.6
En, MeV

Figure 1.

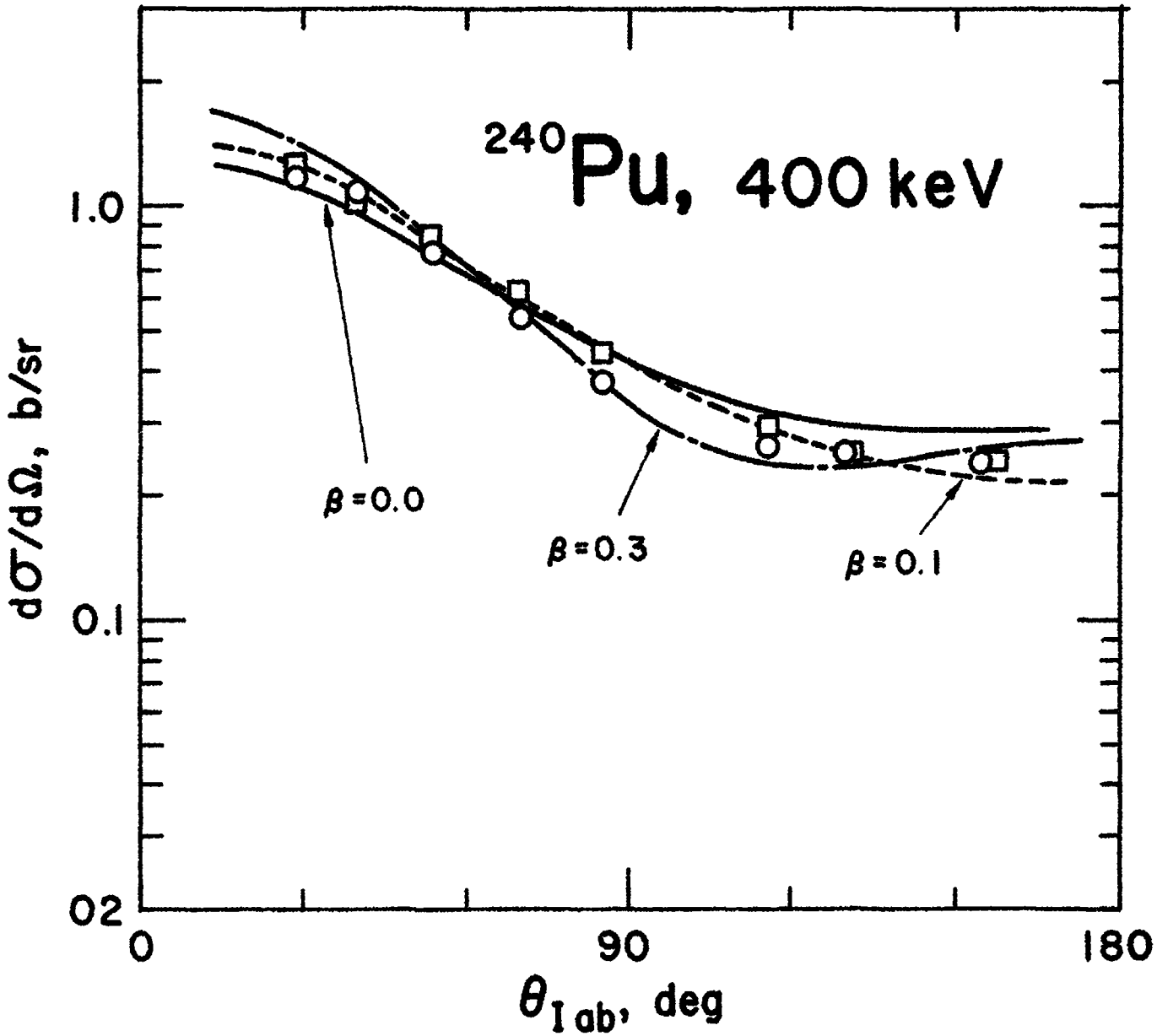


Figure 2-A.

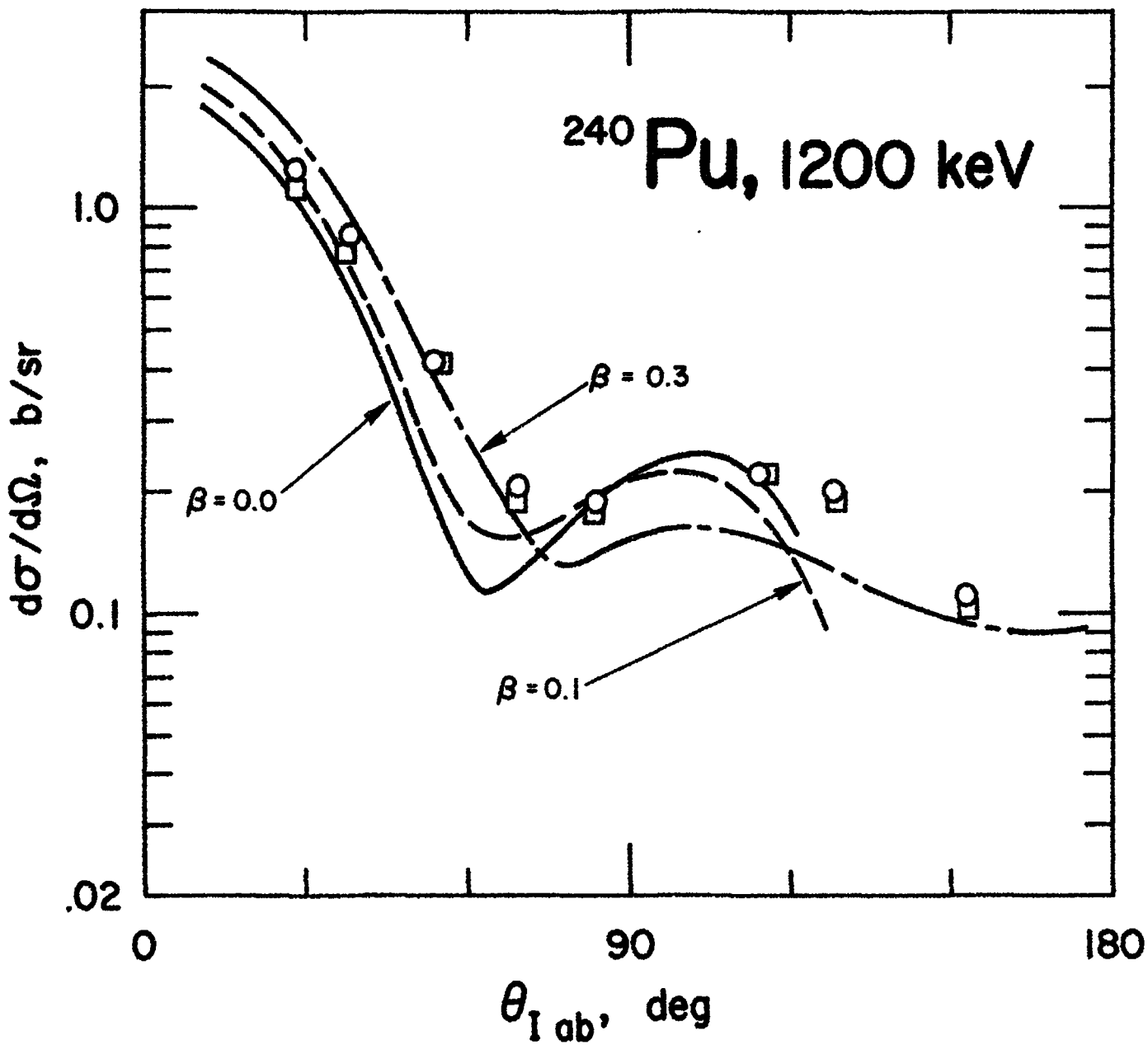


Figure 2-B.

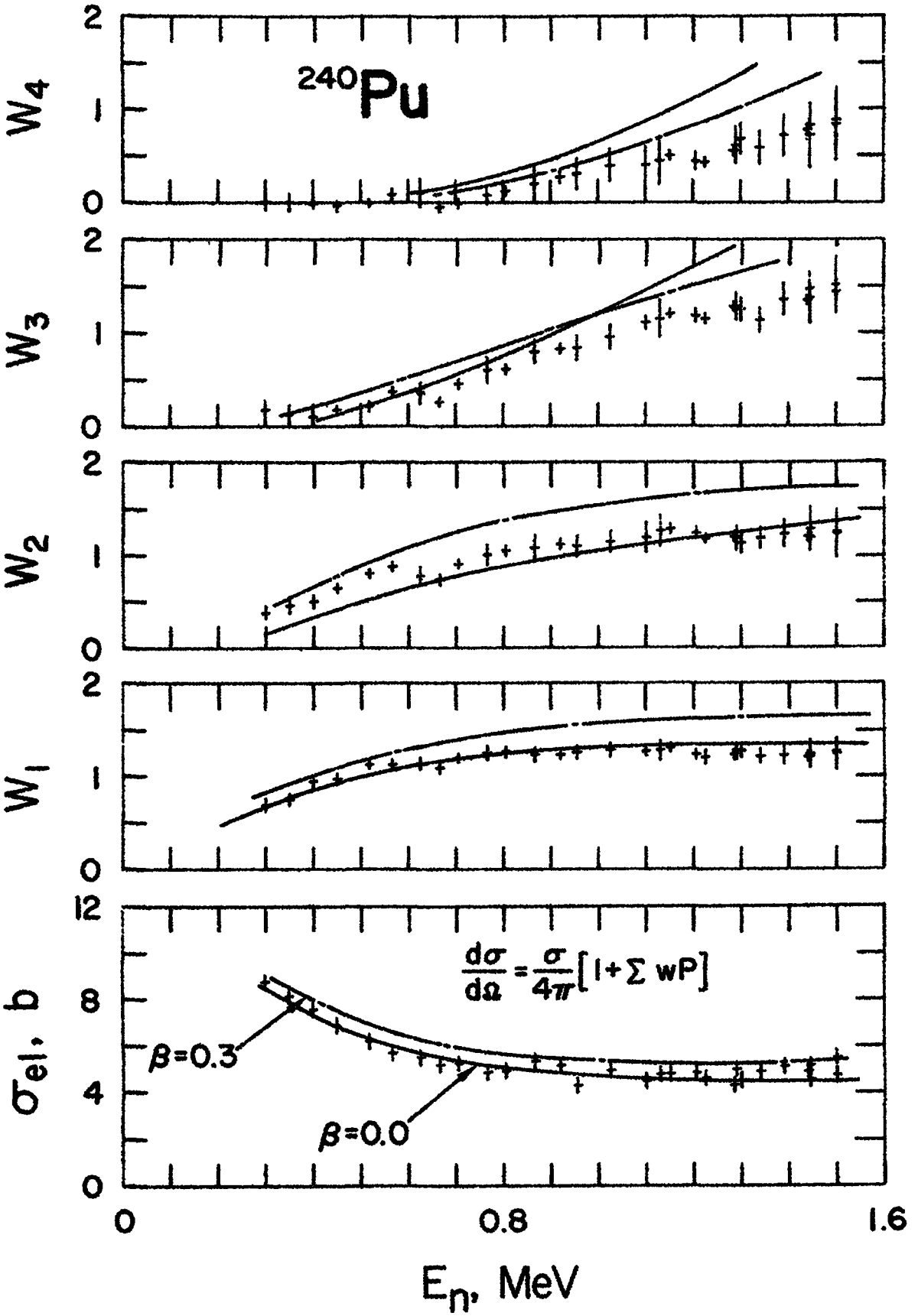


Figure 3.

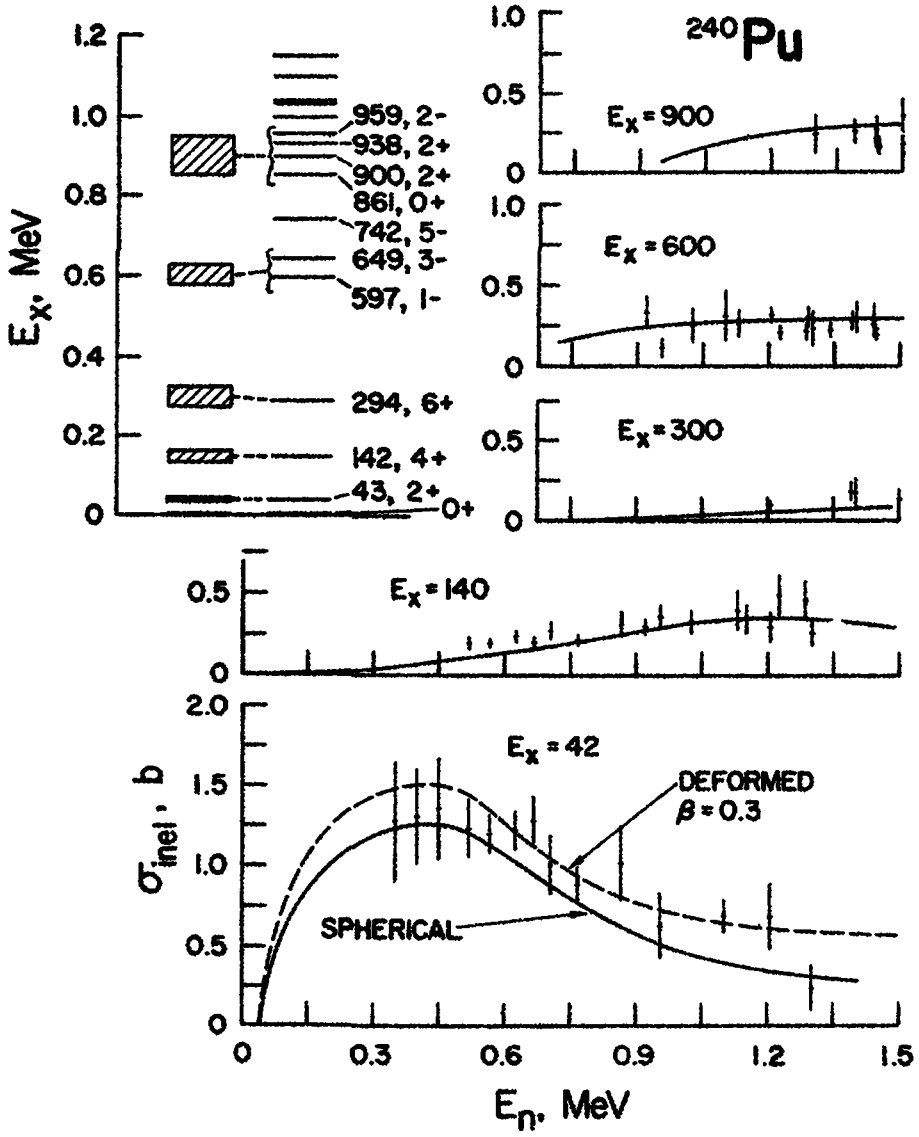

^{240}Pu
E_x, MeV
959, 2-
938, 2+
900, 2+
861, 0+
742, 5-
649, 3-
597, 1-
294, 6+
142, 4+
43, 2+
0+
E_x = 900
E_x = 600
E_x = 300
E_x = 140
E_x = 42
DEFORMED
β = 0.3
SPHERICAL
σ_{inel}, b
E_n, MeV

Figure 4.

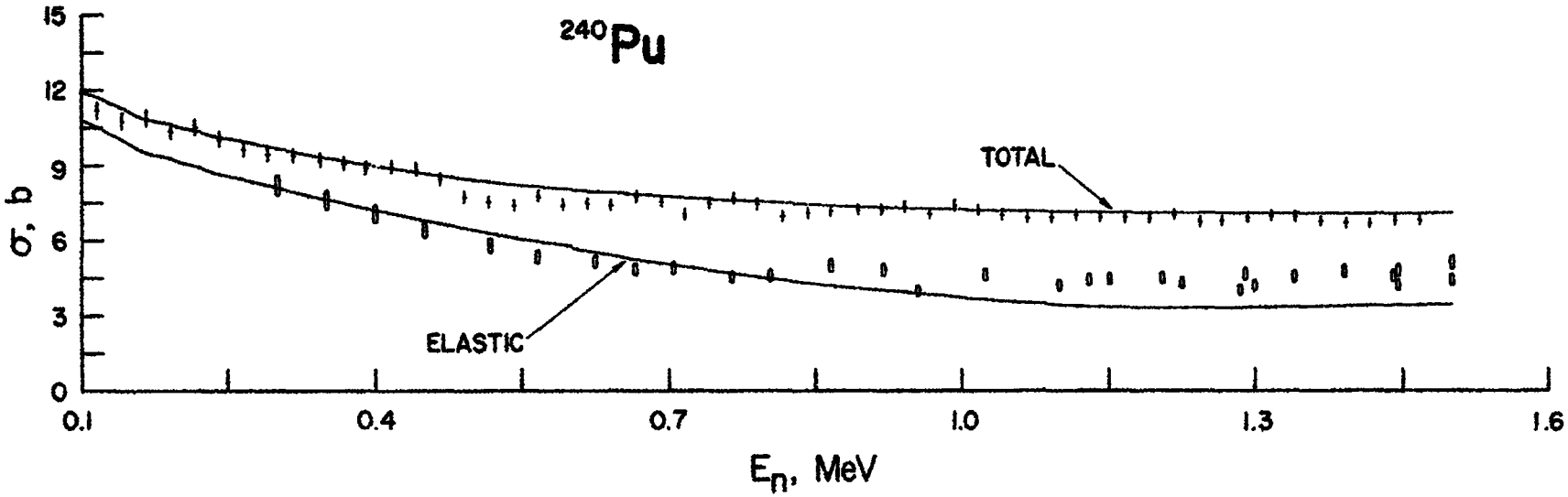
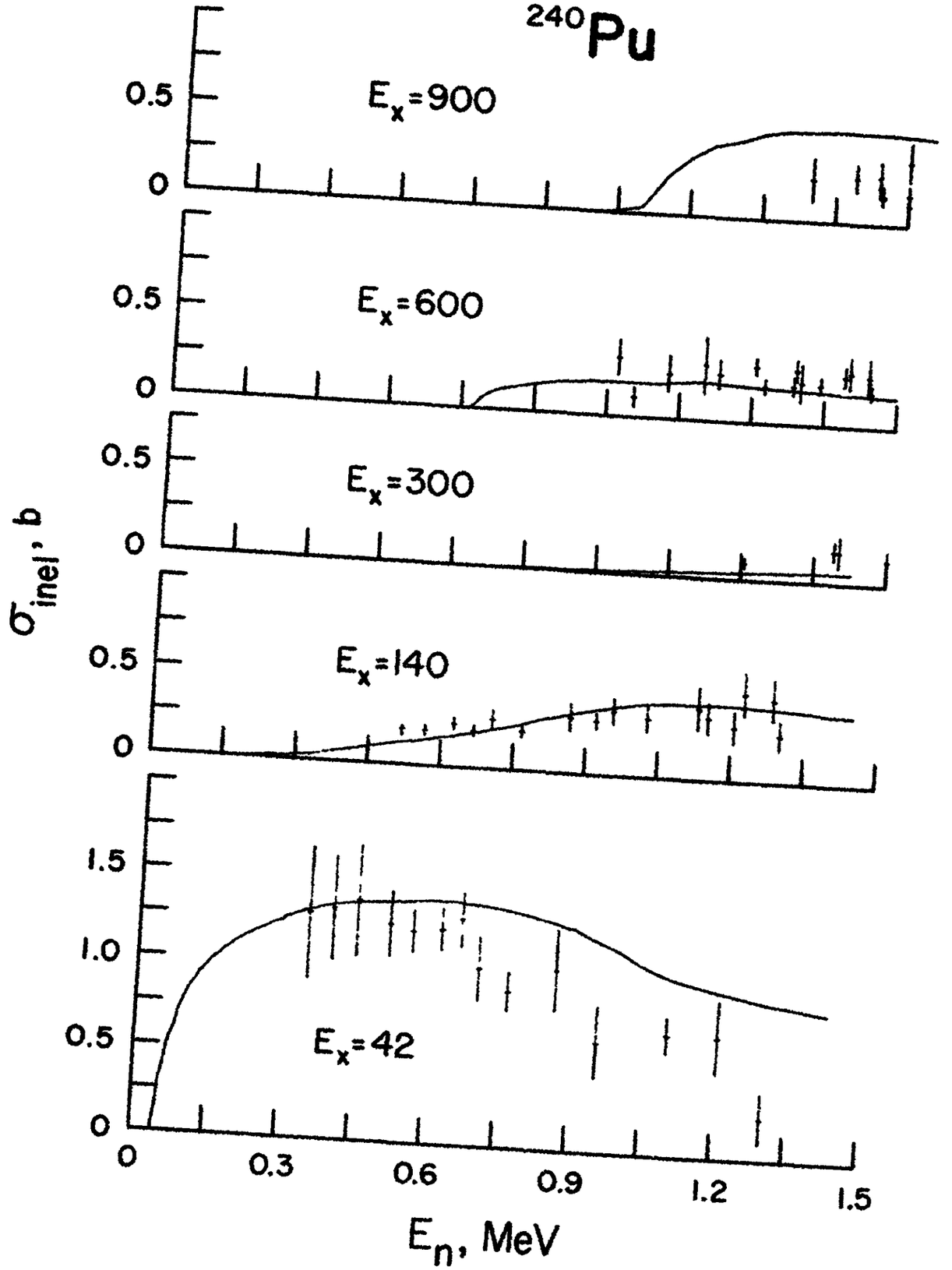


Figure 5.


^{240}Pu
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E_x=600
E_x=300
E_x=140
E_x=42
0.5
0
1.5
1.0
0.3
0.6
0.9
1.2
1.5
σ_{inel}, b
E_n, MeV

Figure 6.

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C     AUTHORS-- A. SMITH AND J. WHALEN, TO BE PUBLISHED                        PU-240
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C     SAMPLE CONTAINED ABOUT 1.3 WT.-PERCENT ALUMINUM, ALL DATA WAS            PU-240
C     CORRECTED FOR THIS CHEMICAL IMPURITY                                     PU-240
C                                                                              PU-240
C     TOTAL CROSS SECTION BLOCK                                                PU-240
C     FORMAT(4E12.6)                                                           PU-240
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C         2. X-SEC IN BARNS                                                    PU-240
C         3. UNCERTAINTY IN X-SEC IN BARNS                                     PU-240
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 .640720E 03 .741123E 01 .222337E 00 .125000E 02                               PU-240
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 .692163E 03 .753130E 01 .225939E 00 .125000E 02                               PU-240
 .716178E 03 .704969E 01 .211491E 00 .125000E 02                               PU-240
 .741694E 03 .748736E 01 .224621E 00 .125000E 02                               PU-240
 .767209E 03 .767075E 01 .230125E 00 .125000E 02                               PU-240
 .791223E 03 .744127E 01 .223238E 00 .125000E 02                               PU-240
 .816737E 03 .694584E 01 .208375E 00 .125000E 02                               PU-240
 .842251E 03 .708674E 01 .212602E 00 .125000E 02                               PU-240
 .867192E 03 .717324E 01 .215197E 00 .125000E 02                               PU-240
 .893774E 03 .721043E 01 .216313E 00 .125000E 02                               PU-240
 .917286E 03 .722770E 01 .216831E 00 .125000E 02                               PU-240
 .940952E 03 .734482E 01 .220345E 00 .125000E 02                               PU-240.
 .966809E 03 .706245E 01 .211873E 00 .125000E 02                               PU-240
 .992321E 03 .737240E 01 .221172E 00 .125000E 02                               PU-240
 .101703E 04 .720687E 01 .216206E 00 .125000E 02                               PU-240
 .104184E 04 .701115E 01 .210335E 00 .125000E 02                               PU-240
 .106738E 04 .691132E 01 .207340E 00 .125000E 02                               PU-240
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.1097187E 04 .6915066E 01 .2074526E 00 .1250000E 02                    PU-240
.1116088E 04 .6991826E 01 .2097556E 00 .1250000E 02                    PU-240
.1140896E 04 .6940796E 01 .2082246E 00 .1250000E 02                    PU-240
.1166640E 04 .6915386E 01 .2074616E 00 .1250000E 02                    PU-240
.1191616E 04 .6887786E 01 .2066336E 00 .1250000E 02                    PU-240
.1216456E 04 .7032366E 01 .2109716E 00 .1250000E 02                    PU-240
.1242716E 04 .6736006E 01 .2020806E 00 .1250000E 02                    PU-240
.1269446E 04 .6797116E 01 .2039136E 00 .1250000E 02                    PU-240
.1291836E 04 .6908936E 01 .2072686E 00 .1250000E 02                    PU-240
.1316456E 04 .6977926E 01 .2093386E 00 .1250000E 02                    PU-240
.1340466E 04 .6937226E 01 .2081166E 00 .1250000E 02                    PU-240
.1365976E 04 .6755266E 01 .2026586E 00 .1250000E 02                    PU-240
.1391386E 04 .6693606E 01 .2008086E 00 .1250000E 02                    PU-240
.1415506E 04 .6678176E 01 .2003456E 00 .1250000E 02                    PU-240
.1441016E 04 .6806696E 01 .2042016E 00 .1250000E 02                    PU-240
.1466516E 04 .6780786E 01 .2034246E 00 .1250000E 02                    PU-240
C                                                                      PU-240
C    END TOTAL CROSS SECTION BLOCK                                     PU-240
C                                                                      PU-240
C                                                                      PU-240
C                                                                      PU-240
C    ELASTIC SCATTERING CROSS SECTION BLOCK                            PU-240
C    FORMAT(6X,214,5(15,14))                                           PU-240
C        1. ENERGY IN KEV                                              PU-240
C        2. X-SEC*100 IN BARNS                                         PU-240
C        3. OMEGA-1                                                    PU-240
C        4. UNCERTAINTY IN OMEGA-1                                     PU-240
C        5 OMEGA-2                                                     PU-240
C        ---                                                           PU-240
C        ---                                                           PU-240
C        ECT., THROUGH OMEGA-5                                         PU-240
C    WHERE-----                                                        PU-240
C        X-SEC IS IN LEGENDRE EXPANSION IN LAB. SYSTEM OF THE FORM     PU-240
C        D=X-SEC/SR.*(X-SEC/4*PI)*(1+SUM(OMEGA-N*P(N)))                PU-240
C    INCIDENT RESOLUTION 20 KEV                                        PU-240
C    SCATTERED RESOLUTION  1.5 NSEC/M                                  PU-240
C    METHOD TIME-OF-FLIGHT                                             PU-240
C    CORRECTED FOR INELASTIC COMPONENT WHERE NECESSARY                 PU-240
C    CORRECTED FOR MULTIPLE SCATTERING                                 PU-240
C    TYPICAL MEASURED ANGLES 28,38,68,83,114,129,155 DEG.              PU-240
C                                                                      PU-240
0     300 820  690  70  380  75  178 100    7 100    0  50    0   0   PU-240
0     350 762  750  61  459  92  125 108    0 100    0 100    0   0   PU-240
0     400 708  946  71  504  79  104  70  -20  50    0  50    0   0   PU-240
0     450 643  973  59  645  54  176  52  -37  66   -2  91    0   0   PU-240
0     518 580 1129  50  798  50  212  57  -14  50    0  50    0   0   PU-240
0     566 534 1130  58  874  53  368  50   84  64   45  89    0   0   PU-240
0     625 515 1138  67  772 101  356 119  101 151   36 210    0   0   PU-240
0     666 485 1088  58  731  58  259  53  -59  52   -7  58    0   0   PU-240
0     705 491 1199  54  905  51  452  55  -14  51  -56  54    0   0   PU-240
0     766 455 1258  78 1001 118  598 138   80 105   35 144    0   0   PU-240
0     805 460 1267  58 1047  57  606  52  121  51  -19  57    0   0   PU-240
0     866 500 1236  78 1077 141  795 127  200 211   49 222    0   0   PU-240
0     920 483 1240  52 1120  59  824  57  273  73  114 101    0   0   PU-240
0     955 401 1264  76 1099 115  831 135  308 172  100 100    0   0   PU-240
0    1025 463 1289  78 1145 118  951 138  394 175  -43 244    0   0   PU-240
0    1100 420 1275  52 1188 164 1106  75  403 195  150 133    0   0   PU-240
0    1130 445 1286 113 1262 172 1150 202  446 256  -81 256    0   0   PU-240
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C     1151 448 1313  53 1283  55 1203  51  500  52   48  73    0   0    PU-240
C     1205 452 1241  51 1240  63 1183  74  442  94  103 130    0   0    PU-240
C     1225 431 1210  76 1180  54 1149  58  434  56  103  50    0   0    PU-240
C     1285 402 1237  55 1198  58 1280  54  551  56  241 179    0   0    PU-240
C     1290 466 1276  87 1183 132 1285 154  615 196  275 272    0   0    PU-240
C     1300 421 1280  72 1125 109 1250 128  684 162  245 225    0   0    PU-240
C     1340 496 1220  77 1185 117 1132 137  587 174  174 242    0   0    PU-240
C     1390 478 1228  98 1228 148 1360 174  723 220  311 306    0   0    PU-240
C     1440 459 1215  58 1197  53 1352  51  779  65  324  90    0   0    PU-240
C     1445 481 1216  54 1183  52 1473  56  830  52  370  55    0   0    PU-240
C     1445 422 1245 157 1280 238 1378 278  721 353  299 391    0   0    PU-240
C     1500 512 1275 130 1246 197 1444 231  890 293  452 407    0   0    PU-240
C     1500 441 1247 173 1231 263 1515 308  840 391  383 544    0   0    PU-240
C                                                                       PU-240
C                                                                       PU-240
C   END ELASTIC BLOCK                                                   PU-240
C                                                                       PU-240
C                                                                       PU-240
C                                                                       PU-240
C  INELASTIC SCATTERING CROSS SECTION BLOCK                             PU-240
C  FORMAT(7E10.4)                                                       PU-240
C      1. INCIDENT ENERGY IN MEV                                        PU-240
C      2. TOTAL SPREAD OF INCIDENT ENERGY IN MEV                        PU-240
C      3. REACTION Q-VALUE IN MEV                                       PU-240
C      4. +- SPREAD OF Q-VALUE IN MEV                                   PU-240
C      5. CROSS SECTION VALUE IN BARNS INTEGRATED OVER ANGLE            PU-240
C      6. + UNCERTAINTY IN X-SEC IN BARNS                               PU-240
C      7. - UNCERTAINTY IN X-SEC IN BARNS                               PU-240
C  CORRECTED FOR MULTIPLE SCATTERING                                    PU-240
C  METHOD TIME-OF-FLIGHT                                                PU-240
C                                                                       PU-240
 PU-240       Q=    -.042000                                           PU-240
.3500E 00 .2000E-01-.4200E-01 .5000E-02 .1278E 01 .3735E 00 .3735E 00  PU-240
.4000E 00 .2000E-01-.4200E-01 .5000E-02 .1309E 01 .2949E 00 .2949E 00  PU-240
.4500E 00 .2000E-01-.4200E-01 .5000E-02 .1358E 01 .3157E 00 .3157E 00  PU-240
.5100E 00 .2000E-01-.4200E-01 .5000E-02 .1231E 01 .1846E 00 .1846E 00  PU-240
.5660E 00 .2000E-01-.4200E-01 .5000E-02 .1199E 01 .1199E 00 .1199E 00  PU-240
.6250E 00 .2000E-01-.4200E-01 .5000E-02 .1217E 01 .1217E 00 .1217E 00  PU-240
.6660E 00 .2000E-01-.4200E-01 .5000E-02 .1278E 01 .1533E 00 .1533E 00  PU-240
.7050E 00 .2000E-01-.4200E-01 .5000E-02 .1007E 01 .1812E 00 .1812E 00  PU-240
.7660E 00 .2000E-01-.4200E-01 .5000E-02 .8864E 00 .1064E 00 .1064E 00  PU-240
.8660E 00 .2000E-01-.4200E-01 .5000E-02 .1020E 01 .2261E 00 .2261E 00  PU-240
.9550E 00 .2000E-01-.4200E-01 .5000E-02 .6280E 00 .2022E 00 .2022E 00  PU-240
.1100E 01 .2000E-01-.4200E-01 .5000E-02 .6902E 00 .1017E 00 .1017E 00  PU-240
.1205E 01 .2000E-01-.4200E-01 .5000E-02 .6890E 00 .2034E 00 .2034E 00  PU-240
.1300E 01 .2000E-01-.4200E-01 .5000E-02 .2386E 00 .1400E 00 .1500E 00  PU-240
 PU-240       Q=    -.140000                                           PU-240
.5180E 00 .2000E-01-.1400E 00 .1000E-01 .1989E 00 .3977E-01 .3977E-01  PU-240
.5660E 00 .2000E-01-.1400E 00 .1000E-01 .1978E 00 .2967E-01 .2967E-01  PU-240
.6250E 00 .2000E-01-.1400E 00 .1000E-01 .2418E 00 .3627E-01 .3627E-01  PU-240
.6660E 00 .2000E-01-.1400E 00 .1000E-01 .2072E 00 .3109E-01 .3109E-01  PU-240
.7050E 00 .2000E-01-.1400E 00 .1000E-01 .2763E 00 .5526E-01 .5526E-01  PU-240
.7660E 00 .2000E-01-.1400E 00 .1000E-01 .2177E 00 .3483E-01 .3483E-01  PU-240
.8660E 00 .2000E-01-.1400E 00 .1000E-01 .3140E 00 .7850E-01 .7850E-01  PU-240
.9200E 00 .2000E-01-.1400E 00 .1000E-01 .3014E 00 .4522E-01 .4522E-01  PU-240
.9550E 00 .2000E-01-.1400E 00 .1000E-01 .3611E 00 .7222E-01 .7222E-01  PU-240
.1025E 01 .2000E-01-.1400E 00 .1000E-01 .3297E 00 .7253E-01 .7253E-01  PU-240
.1130E 01 .2000E-01-.1400E 00 .1000E-01 .4019E 00 .1206E 00 .1206E 00  PU-240
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.1150E 01 .2000E-01-.1400E 00 .1000E-01 .3475E 00 .8687E-01 .8687E-01  PU-240
.1200E 01 .2000E-01-.1400E 00 .1000E-01 .3014E 00 .9043E-01 .9043E-01  PU-240
.1250E 01 .2000E-01-.1400E 00 .1000E-01 .4940E 00 .1235E 00 .1235E 00  PU-240
.1280E 01 .2000E-01-.1400E 00 .1000E-01 .4647E 00 .1162E 00 .1162E 00  PU-240
.1300E 01 .2000E-01-.1400E 00 .1000E-01 .2669E 00 .8007E-01 .8007E-01  PU-240
 PU-240       Q=     -.300000                                          PU-240
.1200E 01 .2000E-01-.3000E 00 .2000E-01 .9546E-01 .2864E-01 .2864E-01  PU-240
.1350E 01 .2000E-01-.3000E 00 .2000E-01 .1821E 00 .5464E-01 .5464E-01  PU-240
.1400E 01 .2000E-01-.3000E 00 .2000E-01 .1758E 00 .8792E-01 .8792E-01  PU-240
.1500E 01 .2000E-01-.3000E 00 .2000E-01 .1382E 00 .5526E-01 .5526E-01  PU-240
 PU-240       Q=     -.600000                                          PU-240
.9200E 00 .2000E-01-.6000E 00 .2000E-01 .3297E 00 .9891E-01 .9891E-01  PU-240
.9550E 00 .2000E-01-.6000E 00 .2000E-01 .1130E 00 .5652E-01 .5652E-01  PU-240
.1025E 01 .2000E-01-.6000E 00 .2000E-01 .2512E 00 .1005E 00 .1005E 00  PU-240
.1100E 01 .2000E-01-.6000E 00 .2000E-01 .3077E 00 .1539E 00 .1539E 00  PU-240
.1130E 01 .2000E-01-.6000E 00 .2000E-01 .2638E 00 .7913E-01 .7913E-01  PU-240
.1200E 01 .2000E-01-.6000E 00 .2000E-01 .3140E 00 .4710E-01 .4710E-01  PU-240
.1425E 01 .2000E-01-.6000E 00 .2000E-01 .2060E 00 .4120E-01 .4120E-01  PU-240
.1285E 01 .2000E-01-.6000E 00 .2000E-01 .2135E 00 .5338E-01 .5338E-01  PU-240
.1290E 01 .2000E-01-.6000E 00 .2000E-01 .3014E 00 .6029E-01 .6029E-01  PU-240
.1300E 01 .2000E-01-.6000E 00 .2000E-01 .2324E 00 .1046E 00 .1046E 00  PU-240
.1340E 01 .2000E-01-.6000E 00 .2000E-01 .2245E 00 .4490E-01 .4490E-01  PU-240
.1390E 01 .2000E-01-.6000E 00 .2000E-01 .2788E 00 .5577E-01 .5577E-01  PU-240
.1400E 01 .2000E-01-.6000E 00 .2000E-01 .2983E 00 .8949E-01 .8949E-01  PU-240
.1440E 01 .2000E-01-.6000E 00 .2000E-01 .2562E 00 .7687E-01 .7687E-01  PU-240
.1440E 01 .2000E-01-.6000E 00 .2000E-01 .2813E 00 .9847E-01 .9847E-01  PU-240
.1445E 01 .2000E-01-.6000E 00 .2000E-01 .1947E 00 .3894E-01 .3894E-01  PU-240
 PU-240       Q=     -.900000                                          PU-240
.1300E 01 .2000E-01-.9000E 00 .5000E-01 .2386E 00 .1193E 00 .1193E 00  PU-240
.1390E 01 .2000E-01-.9000E 00 .5000E-01 .2554E 00 .7662E-01 .7662E-01  PU-240
.1440E 01 .2000E-01-.9000E 00 .5000E-01 .2110E 00 .6330E-01 .6330E-01  PU-240
.1440E 01 .2000E-01-.9000E 00 .5000E-01 .2685E 00 .8054E-01 .8054E-01  PU-240
.1445E 01 .2000E-01-.9000E 00 .5000E-01 .1687E 00 .5060E-01 .5060E-01  PU-240
.1445E 01 .2000E-01-.9000E 00 .5000E-01 .1554E 00 .4663E-01 .4663E-01  PU-240
.1445E 01 .2000E-01-.9000E 00 .5000E-01 .1615E 00 .4845E-01 .4845E-01  PU-240
.1500E 01 .2000E-01-.9000E 00 .5000E-01 .3542E 00 .1063E 00 .1063E 00  PU-240
.1500E 01 .2000E-01-.9000E 00 .5000E-01 .1727E 00 .5181E-01 .5181E-01  PU-240
.1500E 01 .2000E-01-.9000E 00 .5000E-01 .1162E 00 .3485E-01 .3485E-01  PU-240
                                                                       PU-240
                                                                       PU-240
    END OF INELASTIC BLOCK                                             PU-240
                                                                       PU-240
    ********** END OF PU-240 SET **********                            PU-240
                                                                       PU-240
                                                                       PU-240
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