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FINAL REPORT ON THE REAL-84 EXERCISE

BY:
W.L. ZIJP, É.M. ZSOLNAY*
H.J. NOLTHENIUS, E.J. SZONDI*

* Institute of Nuclear Technics of the Technical University Budapest

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Netherlands Energy Research Foundation ECN

PO. Box 1

1755 ZG Petten (NH)

The Netherlands

Telephone (0)22 16-4949

Telex 57211

ABSTRACT

The main aim of the REAL-84 exercise, organized by the International Atomic Energy Agency in Vienna, was to improve the assessment of accuracies in radiation damage predictions by various laboratories using good quality input data and proper calculation methods. The emphasis was concentrated on radiation damage characterization to reactor pressure vessels and related neutron technology.

The long term aim of this exercise was to strive towards the establishment of standardized metrology procedures and recommended nuclear data for use in spectrum adjustment and damage parameter calculations. In this calculation exercise dealing with seven different neutron spectra the best available input data were used. Also some utility programs were included to facilitate the preparation of input data for the adjustment codes.

This final report presents a discussion on the 44 sets of adjustment results received from 12 laboratories. The comparison of the results of the various spectra showed in most cases a relatively large and unexpected interlaboratory spread. Attention is given to this phenomenon. Also the quality of the input data set and a characterization of covariance matrices is summarized.

KEYWORDS

STEELS
THERMAL NEUTRONS
DAMAGING NEUTRON FLUENCE
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DATA COVARIANCES
CROSS-SECTIONS
NEUTRON SPECTRA
SPECTRA UNFOLDING
DATA PROCESSING
LEAST SQUARE FIT

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0. EXECUTIVE SUMMARY

How well can laboratories predict displacement rates with a neutron spectrum adjustment procedure, based on the generalized least-squares methods?

This question is answered by the international interlaboratory exercise REAL-84.

Aim and execution

The aim of the international interlaboratory exercise REAL-84, organized and analyzed under the auspices of the IAEA, was to determine the state-of-the-art in 1984-1985 of the capabilities of laboratories to adjust neutron spectrum information, based on a set of experimental reaction rates, and to subsequently predict the number of displacements in irradiated steel specimens, as well as the uncertainty of this prediction.

In contrast to the previous REAL-80 exercise it was the intention that the participants of the REAL-84 should apply consistently the generalized least-squares method for their adjustment calculations. The exercise REAL-84 was recommended during an IAEA consultants' meeting in Hamburg (26 September 1984).

REAL-84 was organized by the IAEA and a joint team of evaluators was asked to make the necessary preparations for the IAEA and to continue as a team for the analysis of the results. The joint team consisted of staff members of the Budapest Technical University and of ECN Petten.

Input data

The exercise comprised calculation of displacement and gas production rates (as examples of damage parameters) for seven neutron spectra, i.e.

- 3 data sets for the thermal reactors;
- 2 data sets for fusion spectra;
- 1 data set for the ^{235}U fission neutron spectrum;
- 1 data set for a fast reactor spectrum.

The input data for a spectrum set comprised:

- measured reaction rates;
- calculated input spectra;

both accompanied by their covariance information.

Cross-section libraries with uncertainty information were made available together with a number of utility programs to facilitate the data treatment.

The cross-section library contained also displacement and gas production cross-section data for the materials of interest. The uncertainty information for this type of reactions was based on rough estimates for this exercise, because evaluated covariance matrices were not available.

The input neutron spectra which were applied, are considered to be of good quality, but the spectrum information in the low energy range is in most cases highly uncertain. This large uncertainty is sometimes due to a too broad group structure, and sometimes due to lacking spectrum data (e.g. below 1 eV). Too broad energy groups in the input spectra have also been detected in other regions of the neutron spectra.

The input spectrum covariance matrices were completely defined for the spectra of interest. All these matrices were found to be singular within computer accuracy.

During the preparation of the input data for this exercise, a number of reactions -for which measured reaction rates were available- could not be incorporated because the cross-section values and/or their uncertainties were not readily available.

The number of input reaction rates for the thermal reactor neutron spectra is relatively small, while also specific thermal reactions are lacking. The reaction rate covariances for the various spectra have been evaluated with different methods. In a number of cases relatively large standard deviations are present for measured reaction rates.

Task for participant

The participating laboratories were asked:

- to adjust the input data for the seven spectra of interest;
- to calculate for the adjusted spectrum a number of integral spectrum and damage parameters such as:
 $\phi(E > 0.1 \text{ MeV})$, $\phi(E > 1 \text{ MeV})$, ϕ_{tot} , R_{dpa} , R_{He} , R_{H} , etc.;
- to return these data together with a completed questionnaire.

Results of the exercise

From 12 different laboratories 44 solution sets have been received. Data on the solutions are listed in table 4. This table lists also the adjustment codes which have been applied in the exercise as well as the names of the scientists which have participated.

The analysis of the results gave the following general observations:

- The input of the exercise did not supply recommended weighting spectra in a fine group structure. For this reason the participants had to find an appropriate procedure. From the questionnaire it followed that a variety of different procedures was applied. The different procedures will lead to differences in the final results.
- In a number of cases inconsistencies were detected in the input data set during the adjustment. The participants had to remove the inconsistency, and also in this case a variety of procedures could be applied. This leads of course to the same effect as mentioned above.
- The χ^2 -values of the various solutions calculated with comparable adjustment codes show a relatively large spread. This indicates that the input data sets were not identical. This may be due to the points mentioned above.
- Not all participants supplied the normalization values, but in most cases the reaction rates for input and output spectrum were made available. Using these reaction rates together with the input reaction rates a so called "evaluators normalization constant" was calculated which was defined as the mean of the ratios of the two reaction rates.

The evaluators normalization constant showed also a large spread especially for the input of the adjustment procedure. This will influence the adjustment results.

- The solution spectra show in a number of cases clearly discrepant shapes (fig. 6).
- A comparison of calculated reaction rates for the various solutions shows that there are differences between practically all solutions.
- A comparison of the output covariance matrices of the neutron spectra shows that clear differences are present in the various results. For this comparison the eigenvalues, ranks and condition numbers have been calculated (table 2).

Damage predictions

A comparison of the results of the damage parameters shows that the participants' values have some spread (table 15). In principle, one would expect for the given data set only one unique answer.

A comparison of the uncertainties of the damage parameters which were calculated for the various solutions show also a relatively large spread.

Conclusions

Input data sets

General

The situation with respect to consistency and quality of the input data of this exercise turned out to be disappointing.

The reaction rates of a few spectrum sets were obtained in irradiations where special detector covers were applied for one or more reactions. The presence of these covers was not or too late communicated to the participants.

Spectrum and group structure

For all spectra a finer group structure, especially in the low energy region, but incidentally also in other spectrum regions would have been required to achieve more adequate input spectra.

Spectrum covariances

The uncertainty of the input spectrum was very small for two input data sets. As a result, no realistic spectrum adjustment could be expected in these cases (the well-known fusion spectrum and the spectrum of the CFRMF).

Correlation matrices based on physics calculations were available for five spectra. For the two other spectra artificially created correlation matrices were supplied. In these cases the lack of realistic data will have influence on the results.

All input spectrum covariance matrices were found to be singular within computer accuracy.

Reaction rates and their uncertainties

For some input sets the number of experimentally determined reaction rates was too small for the achievement of optimal results. For a number of sets the uncertainty information was only available in the form of variances. A few sets contained very large uncertainties for particular reactions.

Cross-section data

In a number of cases clearly inadequate values for cross-sections and/or their uncertainties were found in the cross-section libraries derived from ENDF/B-V or IRDF-85. Also particular reaction rates could not be applied in the exercise due to the absence of cross-section and/or uncertainty data.

Output of the exercise

In a number of cases the solutions were given in a group structure different from the one in the input data.

Often a large interlaboratory spread in the calculated input and output reaction rates is observed. This fact indicates the presence of inconsistencies in the input data set and/or reflects the effect of different data treatment and calculation procedures.

Calculation procedures

Most of the calculations were performed by spectrum adjustment codes based on the generalized least-squares procedure. Various procedures for the normalization on the input reaction rates were used by the participants. This led to deviations in the solutions.

Integral (damage) parameters

The absolute values for integral parameters which have been calculated by the various participants, show some spread.

This interlaboratory standard deviation is listed for some parameters in table 15a. Table 15b shows the average of the calculated uncertainty values by the participants. A comparison of the data of table 15a and 15b shows that the interlaboratory spread is not low in respect to the predicted uncertainties.

This means that the total uncertainty for the parameter of interest will be larger than the one predicted by the participants.

It will be clear that the interlaboratory spread can only be reduced by improving the input data and the adjustment process (comprising the extension of the number of activation and/or fission reactions and the improvement of the covariance data in the input data set).

1. INTRODUCTION

The REAL-84 exercise was a follow-up of the REAL-80 exercise [1] and has been organized by the Nuclear Data Section of the International Atomic Energy Agency. The aim of the exercise was to improve the assessment of accuracies in the prediction of radiation damage parameters by various laboratories using good quality input data and proper calculation methods. The emphasis was concentrated on radiation damage parameters for reactor pressure vessels and related nuclear technology. Therefore, the upper limit of the neutron energy range of interest was 20 MeV.

The long term aim of the exercise was to strive towards the establishment of standardized metrology procedures and recommended nuclear data for use in spectrum adjustment and damage parameter calculations. The short term aim was the improvement of information on the adjustment technique and its nuclear data needs.

The joint effort of the participants of the exercise has contributed in solving some basic mathematical and physical problems in the neutron spectrum adjustment procedure for radiation damage purposes.

The scope of the exercise and the input data sets have been described in detail in the information sheets [2] and [3] which were distributed to candidate participants. A series of progress reports (with restricted distribution) with ordered output data of the various contributions were prepared during the course of the exercise and distributed among the participants.

An IAEA consultants' meeting on the assessment of the results of the REAL-84 exercise was held in September 1986 in Budapest to consider among others the progress, the presentation of results and furthermore, physical and mathematical problems encountered [4]. These aspects were also reviewed by the IAEA specialists' meeting held in Jackson, Wyoming, USA, May 1987.

The exercise comprised calculations of damage parameters for seven spectra, i.e.:

- 3 data sets for thermal reactors;
- 2 data sets for fusion spectra;
- 1 data set for the ^{235}U fission neutron spectrum;

- 1 data set for a fast reactor spectrum.

It was expected that the input data sets were composed in such a way that a unique solution could be calculated by the participants with a generalized least-squares adjustment code. The evaluation of the results of the REAL-84 exercise was done by a joint team from the Institute of Nuclear Technics of the Technical University Budapest and from the Netherlands Energy Research Foundation ECN.

2. INPUT DATA

2.1. Aspects of the exercise

The participants were asked:

- to use adjustment codes which explicitly can treat covariance matrices;
- to perform well defined neutron spectrum adjustments;
- to evaluate displacement rates and gas production rates for steel samples, when irradiated in these spectra;
- to provide uncertainty and correlation data for parameters of interest;
- to specify the data treatment procedures followed.

Since it was required to use the input covariance information the number of participants was limited. In the preparation of the input sets for the REAL-84 exercise it was tried to obtain data of good quality for the various spectra.

Emphasis was laid on the use of realistic input data. Therefore, several discussions with a few experts in this field took place and their special contributions were added to the available literature data in the specification of the input data sets.

Due to the tight time schedule the enquiries and tests for the input sets had to be finished rather early, with the consequence that a few shortcomings remained in the input data. On the other hand, there were several objective difficulties - for example lack of data and procedures which are based on sound physics or experiments - leading to consequences to be taken into account during the evaluation of the results.

2.2. Spectra investigated

Seven different neutron spectra were used in the input data set of the exercise. Plots of the spectra are shown in fig. 1a ... 1n. The input data sets concerned:

1. ANO: Pressure vessel cavity of the Arkansas Power and Light Reactor (Arkansas Nuclear One-1).
2. PS1: Oak Ridge Research Reactor Poolside Facility in the metallur-

- gical irradiation experiment (position simulated surveillance capsule).
3. PS2: Oak Ridge Research Reactor Poolside Facility in the metallurgical irradiation experiment (1/4 T position in the simulated pressure vessel capsule).
 4. RTN: Fusion simulation spectrum measured at the RTNS-II, a 14 MeV neutron source at Lawrence Livermore Laboratory. (The spectrum is a pretty fair simulation of a first wall spectrum of a fusion reactor).
 5. TAN: Accelerator spectrum Be(d,n) with deuteron energies of 16 MeV.
 6. U35: Fission spectrum of ^{235}U .
 7. CFR: Neutron spectrum in the centre of the Coupled Fast Reactivity Measurement Facility (CFRMF).

2.3. Input data sets

The input data sets were distributed to candidate participants on a magnetic tape by the IAEA. The input data comprised for each set:

- measured reaction rates;
- calculated input spectra;

both data files were accompanied by their covariance information.

Cross-section libraries with uncertainty information and a number of utility programs were also included on the tape. The cross-section libraries contained the cross-section data for all (activation and fission) reactions present in the exercise, and furthermore cross-section data for the calculation of damage parameters such as the number of displacements and gas production.

Covariance information was available in the cross-section library for all reactions of interest, except those needed for the damage characterization. To fill this gap, artificial uncertainties were introduced. Of course, these data have a meaning only for comparison purposes in the exercise since they lack all physics background. More information on the input data sets is given in table 1.

3. QUALITY OF THE INPUT DATA

3.1. Input neutron spectra

The input neutron spectra which are applied in the exercise are considered to be of good quality, but the spectrum information in the low energy range is highly uncertain in most cases (see also fig. 1). In some cases this large uncertainty is due to a too broad group structure in this energy range (for example PS1, PS2, TAN, RTN and U35), and sometimes due to lacking spectrum data below about 1 eV (for example ANO and CFR).

Similar problems (i.e. too broad energy groups in the input spectrum) can be encountered also in other energy ranges of the spectra, for example in the keV region of the CFR, where (n, γ) reactions have their responses, and in the high energy range where the (n,2n) reactions are sensitive. The shortcomings of the input spectrum information lead to difficulties in the adjustment and in the calculation of the characteristic integral spectrum- and damage parameters such as fluence rate values and dpa rates.

3.2. Cross-section data

The reaction cross-section data for the exercise were derived from the best available up-to-date compilations such as the second version of the dosimetry and gas production file of the ENDF/B-V [13] and the IRDF-85 [14]. Nevertheless during the preparation of the input data sets a number of reactions - for which measured activities were available - could not be incorporated because the cross-section data were not readily available.

This lack of reaction cross-section data together with their uncertainties is in a few cases the reason of a restricted number of reactions in the REAL-84 input data sets. The reactions with lacking cross-section uncertainty information were:

$^{45}\text{Sc}(n,2n)^{45}\text{Sc}$, $^{52}\text{Cr}(n,p)^{52}\text{V}$, $^{54}\text{Fe}(n,\alpha)^{51}\text{Cr}$, $^{64}\text{Zn}(n,\gamma)^{64}\text{Zn}$,
 $^{60}\text{Co}(n,p)^{60}\text{Fe}$, $^{88}\text{Y}(n,2n)^{88}\text{Y}$, $^{93}\text{Nb}(n,\gamma)^{93}\text{Nb}$, $^{93}\text{Nb}(n,2n)^{92}\text{Nb}$,
 $^{109}\text{Ag}(n,\gamma)^{109}\text{Ag}^{\text{m}}$, $^{168}\text{Tm}(n,2n)^{168}\text{Tm}$, $^{197}\text{Au}(n,2n)^{196}\text{Au}$ and
 $^{238}\text{U}(n,2n)^{237}\text{U}$.

The majority of these reactions is of special interest for fusion neutron metrology. For a number of these reactions evaluations are available which are not yet incorporated in the metrology cross-sections libraries. Discrepant cross-section values were found by several participants for a number of reactions, for example:

$^{48}\text{Ti}(n,p)^{47}\text{Sc}$, $^{59}\text{Fe}(n,\gamma)^{60}\text{Fe}$, $^{60}\text{Ni}(n,2n)^{59}\text{Ni}$ and $^{127}\text{I}(n,2n)^{126}\text{I}$.

Furthermore, the $^{115}\text{In}(n,\gamma)^{116}\text{In}$ reaction cross-section had to be calculated from the total (n,γ) cross-section data given in the ENDF/B-V version 2 dosimetry file.

3.3. Damage and gas production cross-sections

In the input data damage cross-section values for three different materials (Fe, Cr and Ni) were supplied. These displacement cross-section values were made available so that the participants could calculate the displacement rate for the specified (REAL-84) steel (i.e. 71% iron, 18% chromium and 11% nickel).

One can doubt whether a linear combination of the components' displacement cross-sections (method presently used in practice) will constitute the total displacement cross-section for the given type of steel. Nevertheless new developments in this field indicate that no large differences in damage cross-sections can be expected when calculated by the linear combination of components or by a more sophisticated method which directly considers the damage in the steel of interest. More information on this subject is given in [4a] and [15].

In order to calculate the production rates of helium and hydrogen gas in the steel of interest the ENDF/B-V gas production cross-sections were also available (IRDF-85 library) ([13] and [14]).

3.4. Input reaction rates

The input data sets for the thermal reactor neutron spectra have in all the three cases a small number of reaction rates (see fig. 1a ... 1d). Also in all cases the thermal neutron response is lacking. It seems a poor situation that the input data sets on one side have a small number of experimental reaction rates while on the other side a significant effort has been made to obtain realistic covariance

information for these data and to use advanced adjustment methods. From this point of view an intensified effort for improvement of the metrology information seems to be justified.

3.5. Input spectrum covariances

For the REAL-84 exercise the spectrum covariances were completely defined. The covariance information for the ANO cavity position is available in 16 groups while the spectrum is given in 55 groups. This covariance matrix and the spectrum were calculated and made available by Dr. R.E. Maerker (ORNL). A plot of these data is given in fig. 3.

The uncertainty information for the PS1 and PS2 (PS1 is the surveillance position, and PS2 is the 1/4 T position in the metallurgical irradiation experiment) was identical. As these input data sets represent different irradiation locations also different covariance matrices can be expected. The large uncertainties in the low energy groups (standard deviation larger than 100%) show that improvement of the data is required. The pool side facility data were supplied by Dr. F.W. Stallmann (ORNL). The covariance matrix was based on calculations by Dr. R.E. Maerker. An extrapolation of this matrix to the low energy region was made by Dr. F.W. Stallmann.

The covariance matrices for the fusion type spectra were based on calculated variances and in lack of calculated data, on artificial correlation matrices with a Gaussian shape.

For the reference spectra (U35 and CFR) the uncertainty information comprised such small values that no real improvement of the neutron spectra could be expected. Fig. 4 shows the input spectrum covariance matrix for the U35 set.

The input spectrum (and cross-section) covariance matrices in the group structure of interest do not fulfil the requirements of covariance matrices in the sense of mathematical statistics (see appendix). The matrices are not "positive definite" ones. Calculations have shown that all of them were singular within computer accuracy (see table 2). This indicates physically that the relations between the different variables (group fluence rates or group cross-section values) are not described adequately in the group structure which was applied.

The quality and the condition of the input spectrum covariances for a series of different neutron spectra need to be investigated both from a physics and mathematics point of view. Especially because this spectral uncertainty seems to be crucial information for generalized least-squares adjustments.

3.6. Cross-section covariances

Cross-section covariance information was available for all metrology reactions in the IRDF-85 [14] and ENDF/B-V [13] dosimetry libraries. For several reactions the uncertainties calculated from the library were so large that they resulted in a negligible statistical weight for the reaction of interest in the adjustment procedure.

Also the too coarse original group structure of the uncertainty information with large jumps in the uncertainty values seems to be unrealistic (for example $^{197}\text{Au}(n,\gamma)$ in fig. 5). In the group structures of interest in the exercise all the cross-section covariance matrices were found to be singular within computer accuracy.

From the data in table 3 and fig. 2 it can be concluded that the reaction rate uncertainties calculated for the various spectra are sometimes relatively large with respect to other reaction rates in the same set. This is caused by their large cross-section uncertainties. In general, reactions with relatively large uncertainties will not contribute much information in the adjustment when also reactions with small uncertainty data are applied.

Another phenomenon which indicates that the large uncertainty values in the cross-sections are a disadvantage, can be illustrated by the reaction $^{47}\text{Ti}(n,p)$. It is well known that the cross-section data for this reaction are incorrect. Simultaneously these erroneous data are accompanied by large uncertainty values. As a result, the contribution of this reaction to the χ^2 -value in a least-squares adjustment is relatively small, and it does not show the presence of an incorrect cross-section value. However, practically all participants detected it.

In a few cases cross-correlations between different reaction cross-section sets occur. These data were not used by the participants. The influence of neglecting these cross-correlations on the results cannot be estimated but it is supposed to be small.

Experimental uncertainty data for the damage producing reactions is not available at this moment. Uncertainty values have been arbitrarily chosen for the displacement and gas production cross-sections, so they have only meaning for comparison purposes. The uncertainty values chosen are 10% for iron, 12% for nickel and 18% for chromium for each group.

It was assumed that the correlation between the various groups could be described by means of a special Gaussian function (for details see [3]).

3.7. Reaction rate covariances

The reaction rate covariance matrices available in the exercise originate from different evaluation methods. Agreement should be reached on the best method to calculate these data. In a number of cases the standard deviations of the measured reaction rates are relatively large: for example for all reactions of ANO, for the fission reactions in PS1, 3 reactions in TAN, RTN and U35. The reason of the 500% standard deviation for the reaction U238F in the PS1 is not clear.

3.8. Detector covers

In a number of cases, special detector covers were applied during the irradiations (Boron in ANO, cadmium in RTN and gadolinium in PS1). Unfortunately, not enough attention could be paid to this subject in the preparation of the input data for the exercise. A letter with additional data did not reach all participants in time.

Nevertheless, the correction for the influence of a detector cover on the detector response is not a straight forward procedure at this moment, especially if also the uncertainty of the corrections has to be taken into account.

3.9. Role of the group structure in input data

The calculated neutron spectra were available in various group structures (from 24 to 60 groups). In most cases the given group structures were used directly in the adjustment calculations. In one case (ANO) the spectrum covariance matrix was given in 16 groups while the spectrum was available in 55 groups. Here a conversion was required. In a few cases the spectrum was reduced to 16 groups but in most cases the covariance matrix was extended to 55 groups.

It has been remarked already in section 3.1 that the group structure was not completely satisfactory in certain spectral regions. Difficulties were met in the definition of a detailed smooth weighting spectrum which is needed in the derivation of group cross-section values and their uncertainties.

At this moment no recommended working method is available and this led to a variety of procedures, which evidently had an effect on the results. In a few cases extra information, not present in the exercise, was used while also several mathematical procedures were applied. In the future more attention should be given to the weighting spectrum definition.

Also computer programs for the conversion of covariance matrices from one group structure to another should be made available through the channels of the Nuclear Data Centres.

3.10. Utility programs supplied in the exercise

Several utility programs were included in the exercise for the convenience of the participants. A number of them was intended for data handling from the REAL-84 magnetic tape. Other ones were intended to convert fine group cross-section data to a selected coarse group structure (FITOCO [16] and GROUPIE [17]), to linearize data from an evaluated nuclear data file in the ENDF/B-V format (LINEAR [18]), or to read the uncertainty information from a cross-section library with the ENDF/B-V format and convert these data to a matrix with a selected

group structure UNC33 [19]. To ensure the availability of the program UNC33 in the exercise, it was converted from FORTRAN-77 to ANSI STANDARD FORTRAN.

During the exercise it became clear - also by indications from the participants - that in some parts of the software errors occurred. Also in this case the information on the corrections did not reach all participants in time. Nevertheless, the influence of the software errors on the results of the exercise was not significant; this was shown by comparison of the results, calculated by one laboratory under identical conditions for the uncorrected and corrected software.

4. RESULTS

The analysis of the results comprised 44 solutions obtained from 12 participating laboratories. Table 4 gives a survey of the participating laboratories, their adjustment codes and the supplied solutions. A detailed discussion of the results with a summary for each spectrum was prepared in the form of progress reports with restricted distribution, distributed among the participants.

4.1. Adjustment codes and utility programs

The participants applied various adjustment codes and procedures to calculate the neutron spectrum and characteristic integral (damage) data, together with their uncertainties. Adjustment codes NEUPAC-JLOG [20], LEPRICON [11], LSL-M2 [21], different versions of STAY'SL [22], and SAND-II [23] (SANDBP [24] and SANDMX [25]) were used (see table 4).

In most cases no detailed information on the differences between the STAY'SL versions is available. The cross-sections and their uncertainty information were converted by the participants from the ENDF/B-V format to the group structure of interest with aid of the programs NJOY [26], PUFF-2 [27] or UNC33 [19]. One participant used systematically the standard deviations of the ENDF/B-V file in combination with Gaussian shaped correlation contributions, instead of the library correlation matrices.

For the conversion of covariance matrices no special programs were mentioned by the participants.

4.2. The weighting spectra

For the calculation of the group cross-sections and the covariance matrices of these values, a weighting spectrum in a fine group structure or in a continuous form was needed. The input of the exercise did not give this spectrum or a recommended procedure to obtain this spectrum. For this reason the participants had the freedom to find an appropriate procedure for this purpose. A variety of procedures was applied, for instance:

- more detailed evaluations of the spectra from other sources were applied (more detailed calculations or theoretical functions);
- simple functions different from the actual spectra (thermal Maxwellian, $1/E$ and Watt fission spectrum);
- interpolation and extrapolation of input spectrum data;
- application of the coarse spectrum in a fine group structure.

In the interpolation and extrapolation procedure various methods were applied, for example log-log interpolation, special spline methods, etc. The difference due to the weighting spectra can be observed in the reaction rates calculated for the input spectra by the various participants (see table 5).

4.3. The treatment of inconsistencies

During the adjustment procedure the participants detected various inconsistencies in the input data sets. These inconsistencies were detected by an unacceptable value of the χ^2 -parameter or by too large differences of measured and calculated reaction rates. No methods to remove the inconsistencies were recommended and for that reason the participants had much freedom to modify their input sets.

A variety of actions to obtain consistency in the input data set was taken:

- one or more reaction rates were deleted from the input;
- the standard deviation of one or more reaction rates were changed;
- the input spectrum was changed in one or more groups, extrapolated, etc.;
- the variances of a part of the input covariance matrix were changed.

The different procedures which were applied for the correction of the inconsistencies led actually to the definition of a series of input data sets which were different and thus resulted in different output data.

4.4. The χ^2 -values for the various solutions

The χ^2 -value calculated for the input data can be applied for the judgement of the consistency, while also the χ^2 component for each

separate reaction can be helpful in the investigation of the quality of the input data set. The definition of this parameter is given by F.G. Perey [22].

For the sake of comparison the χ^2 -value per degree of freedom was calculated from the participants data. The maximum and the minimum values for the various spectra are given in table 6. In this table only STAY'SL version solutions were considered. One would expect the same χ^2 -value for all solutions of a given input data set. But the table shows that a large range of χ^2 -values was obtained. Of course, it should be taken into account that in several cases the participants performed modifications in the input data to achieve improved consistency.

In general it can be concluded that the solutions which were received did not indicate inconsistencies in the supplied input data sets, but the large spread in the results shows that there are differences both in the input data and in the calculation methods.

4.5. The normalization of input and output spectrum

Not all participants supplied the normalization values in their solutions, but in most cases the reaction rates for input and output spectrum were made available. Furthermore, they used various definitions for the normalization. For this reason the evaluators calculated a normalization constant for the various solutions. This constant was calculated according to the relation:

$$F = \frac{1}{n} \sum_i \frac{A_i^p}{A_i^m}$$

where:

F = evaluators' normalization constant;

n = number of reaction rates;

A^p = participants' reaction rate;

A^m = measured input reaction rate.

This normalization constant has been calculated for the participants' input and output reaction rate sets. Table 7 shows the average value and the spread in F for the various input data sets.

The results show that especially the input normalization yields a large spread which will influence the adjustment results. A consequent application of the normalization procedure as described elsewhere [28], preceded by a rough scaling, would certainly reduce the spread.

4.6. The solution spectra

The modifications of the input data set because of inconsistencies and differences in calculation procedures, which were described, led to clear discrepant output spectra of the various adjustments. In fig. 6 plots are given which show a comparison of various solution spectra. It should be remarked that not for all solutions the output spectra were available.

4.7. The calculated reaction rates

The calculated reaction rates accompanying the solutions have also been compared. Two methods have been applied for this comparison:

- Ratios of A_i^P/A_i^m (indicated in the table as C/E) have been calculated. An example is given in table 8. The A_i^P values were calculated for the output spectrum;
- Normalized ratios of measured and calculated reaction rates have been calculated with the relation:

$$Q_i = \left(1 - \frac{1}{F} \cdot \frac{A_i^P}{A_i^m}\right) \times 100$$

Examples of these normalized reaction rate ratios (Q) are given in table 9 for the input and in table 10 for the output spectrum. The calculation results show that differences exist between practically all solutions for the input as well as for the output reaction rates. In the case these ratios (Q) are divided by their standard deviations no significant values can be detected for the majority of the solutions. On the other hand, for all solutions it can be observed that some reactions have relatively high differences and calculated reaction rates with respect to the other reactions. For example the reaction $^{47}\text{Ti}(n,p)$.

4.8. The calculated reaction rate uncertainties

Reaction rate uncertainties were also present in the solutions. Plots of these data (fig. 2) show the contribution of different terms (i.e. measured reaction rate, cross-section and spectrum) to the uncertainties of the reaction rates. In the plots also the uncertainty contribution of the output spectrum can be seen. For purpose of demonstration a STAY'SL type output was used.

In the adjustment codes the reaction rates have been calculated by means of group fluence and group cross-section values. The uncertainty in the reaction rates is derived from the contribution of the group cross-sections and the group fluences using the law for the propagation of uncertainties. In the derivation of the uncertainties with this law a function is obtained which contains also non-linear terms. In general, these higher order terms are neglected. In this case a more exact uncertainty value for the reaction rate can be derived by adding a restricted number of cross-product terms ($s_{\text{non-linear}}$) to the usual relation without higher order terms. Details on the derivation of this method are given in [1]. In table 11 a summary is given for the contribution of the non-linear terms to the total uncertainty of the calculated reaction rate. This "relative contribution" is expressed as follows:

$$s_{\text{non-linear}} \times 100 / (s_{\phi}^2 + s_{\sigma}^2 + s_{\text{non-linear}}^2)^{\frac{1}{2}}$$

where:

- $s_{\text{non-linear}}$ = contribution of non-linear terms;
- s_{ϕ} = contribution of uncertainty of the spectrum;
- s_{σ} = contribution of uncertainty of the cross-section.

Also the influence of these terms on the variance is shown. The ratio of the variances calculated with the contribution of non-linear terms is given in table 11.

4.9. The covariance information for the solution spectra

Covariance matrices for the solution neutron spectra were analysed. The eigenvalues were calculated and some characteristic data (effective rank, condition number) were derived. For demonstration purposes

characteristics for the correlation matrices are shown in tables 2a ... 2g. In line 9 of the tables the decimal logarithm of the condition number (i.e. ratio of the highest and smallest absolute value of eigenvalues) is given. The more the condition number deviates from unity (i.e. its logarithm from zero) the more ill-conditioned is the correlation matrix.

Covariance data supplied in SET 3 were not analysed since band matrices for the cross-sections were used in this case and the group structure of the output data deviates also from the common group structure of the other solutions. For this reason the covariance data are not easily comparable.

The effective rank both for the input and the output covariance matrices lies between one half and one quarter of the number of groups of the spectra (see tables 2a ... 2g). It means that only this proportion of the matrix yields non-redundant uncertainty information. Owing to the singular character of the covariance matrices, no inversion of these matrices is possible. Fortunately, the formulae for the calculations of the adjusted parameters and their variances with the linearized least-squares model require only the inversion of the matrix $[\underline{V}(A^C) + \underline{V}(A^M)]$.

Fortunately in practical cases this matrix turns out to be non-singular. Due to the ill-conditioning of this covariance matrix, the output of the adjustment procedure may yield negative "variances". One participant observed this phenomenon in case of the ^{235}U fission spectrum, which actually is a reference spectrum. The situation becomes remarkable when the reference spectrum is characterized by a singular matrix. Consequently, further developments in this field also for the ENDF/B-V library are needed. More detailed information on this subject is presented by Dr. M. Matzke in [29].

Numerical difficulties (rounding problems) in the calculation procedures with these matrices were encountered in most cases as both the input and output covariance values were reported rounded to 2 or 3 digits. In case of the spectrum CFR a clear mistake in the output covariance matrix was detected: for one of the correlation coeffi-

cients a value of 1.015 was obtained in all the solutions, which cannot be interpreted as rounding error. The reason for this mistake may be due probably to the large number of negative eigenvalues present in the matrix, or may be produced by the linearized estimate of the STAY'SL code [22] in case of ill-conditioned input covariance matrices.

In general, the rank of the output covariance matrices is higher than the one for the input. In case of STAY'SL type codes theory shows that the rank of the output fluence rate covariance matrix has to be lower than or equal to the rank of the input matrix [4a]. Any increase of the rank by the adjustment procedure - as observed for the solutions - corresponds to the addition of non-relevant information to the spectrum by the computing procedure.

The input spectrum covariance matrix for ANO was found to be singular (within computer accuracy) already in the 16 groups representation. As most of the calculations were performed in 55 groups, the given covariance information had to be converted ("blown up") to this finer group structure thus developing a matrix being also theoretically singular. On the other hand, also the calculations in 16 groups are not satisfactory due to the poor spectrum representation.

5. SUMMARY OF DAMAGE PREDICTIONS

5.1. Integral (damage) parameters

The aim of the exercise was to obtain an impression of the interlaboratory differences in the estimates for the integral (damage) parameters and their uncertainties used in the lifetime assessment of reactor pressure vessels in order to arrive at better and reproducible methods. Ideally, one would like to obtain for the given data set only one unique answer, i.e. one unique final parameter value with one final value for its standard deviation. Nevertheless, the comparison of the results shows that the participants' values have some spread. Differences in the outcomes might be due to differences in mathematical-statistical procedures (rounding uncertainties, word length, matrix inversion procedures, optimization procedures, etc.) or in modifications based on the physics (group structure, spectrum extrapolations, deletion of reaction rates, modification of covariance matrices, introduction of other cross-section sets, etc.). When considering the participants' responses one should keep in mind that these results do not constitute independent data, since they are all based on the same input set of observations.

The results of the REAL-84 calculational procedure yield a set of parameters together with their uncertainties that describe the characteristics of the irradiation of the materials of interest (steel). The parameters currently used for this purpose are neutron spectrum characteristics and typical parameters which are considered to have a more direct relation to the damage processes.

These parameters comprise the displacement rate and the production rate of helium and hydrogen atoms. Of course, for the actual irradiation experiments an integration of the parameters of interest over the time is required. It is repeated here that the calculated uncertainties in the damage parameters are based partly on artificial uncertainty data.

In order to facilitate the comparison, the results of these parameters together with their standard deviations are presented in plots for

the various input data sets (fig. 7a ...7g). In the plots the results obtained for the parameter of interest is ordered in increasing value. The left y-axis shows the actual value of the parameter. The right y-axis contains a percentage scale for an easy comparison. The values along this scale are intended to show the magnitude of the differences of the data but do not have an absolute sense with respect to a reference value.

The horizontal lines in the plots indicate the interlaboratory average and standard deviations. In the calculation of these values all participants' values were considered to have the same statistical weight. From the plots it can be seen that not all participants gave all parameters, and in a number of cases the uncertainty data were lacking.

The interlaboratory standard deviations are even larger than the comparable values found in the preceding REAL-80 exercise [1]. A reason might be that the consistency of the input data of the REAL-80 exercise was better than that of the REAL-84 input data set. Nevertheless, one should not forget that in the REAL-80 exercise artificial covariance data (band matrices, defined by analytical functions) were used, while the REAL-84 data set is considered to contain improved physical information, especially for the uncertainties.

5.2. Uncertainties in integral data

The benefit of the adjustment procedure is reflected in the decrease of the uncertainties in the integral spectrum and damage parameters.

For a demonstration of this merit some uncertainty data are given in tables 12 and 13, which have been calculated for the input spectrum data (without adjustment) and with the output spectrum data (after adjustment). From these tables it can be seen that for the thermal reactor spectra a decrease of the uncertainty by about a factor 2 is obtained. For the fusion type spectra the decrease of the uncertainty is between a factor 3 and 4. For the two reference spectra (U35 and CFR) no significant decrease is found. The uncertainty of these input spectra is so low, that the reaction rates cannot contribute extra information due to their relatively large uncertainties. In the case of the U35 data set numerical problems were encountered by one participant due to properties of the input covariance matrix.

It should be realized that the decrease of uncertainties given in the tables does not show the uncertainty contribution due to the normalization procedure performed during the adjustment. In the case that the recommended normalization procedure as described in [1] is applied, then an uncertainty of the normalization factor can also be calculated (10 ... 30%).

In principle this uncertainty should be incorporated in the "before" spectrum covariance matrix.

In a number of cases the uncertainty values of integral parameters determined by the different laboratories show a large spread. Differences by a factor greater than 3 sometimes occur between standard deviations reported by the different participants. For the thermal and intermediate neutron energy region these data have a limited importance due to the rough energy group structure in this part of the spectrum. The observed very large spread in the standard deviation of integral (damage) parameters indicates that they are very sensitive to the different data treatment and calculation procedures. Basically, they are determined by the covariance information of the cross-section and spectrum data applied. Any deviation from the input covariance information specified for the exercise will be reflected by the uncertainty values discussed here.

After adjustment, the spectrum contribution to the standard deviation of the integral data has significantly decreased. Therefore, the uncertainty of the output reaction rates and damage parameters is in most cases determined by the uncertainty contribution of the cross-sections (activation, displacement or gas production). The cross-section uncertainties for the activation reactions derived from the ENDF/B-V file are high for a number of reactions. The uncertainty values for the damage cross-sections were not based on evaluations. Therefore artificial standard deviations (10% for Fe, 12% for Ni and 18% for Cr) were chosen for this exercise.

6. DETAILS FOR THE SPECTRA OF INTEREST

In the following part a discussion is given of the data as returned for the 7 input data sets.

6.1. ANO

The input data set contained 6 experimentally determined reaction rates, a calculated spectrum in 55 groups and fluence rate covariance matrix in 16 groups. The reaction rate for ^{235}U was determined inside a boron cover. The effect of this cover on the ^{235}U fission rate is about 5%. Due to a misunderstanding the presence of the cover was not communicated to the participants. The effect of this omission is thought to be small due to the large uncertainty of the reaction rate of interest (11.8 per cent).

The other uncertainties have also relatively large values. Some participants expanded the covariance matrix to 55 groups or even to 100 groups.

In the fine groups within a coarse group the covariances were assumed to be equal to the covariance of the coarse group. In the conversion to the 100 group structure the same method was applied. In this case the energy boundaries were not equal and therefore the fine group boundaries next to the coarse group boundary were applied and no interpolation of covariances was performed.

The results lead to the following remarks:

- Only SET 2 contained the correction for the boron cover.
- The results of a sensitivity analysis added for SET 1 are shown in table 14. This table shows the various variance components in the derived dpa-values.

6.2. PS1

The input data set contained 10 experimentally determined reaction rates, and the input spectrum and its covariance matrix in a 37 group structure. No detector response was available for thermal neutrons. In a late phase of the exercise it was communicated that all detectors were irradiated in a gadolinium cover. The reaction rate of $^{235}\text{U}(n,f)$ had an uncertainty of 500% in the input. One participant

performed his adjustment calculation with a 5% uncertainty instead for this reaction (SET 5).

The following remark can be made:

- Two participants performed a modification of the input spectrum before starting the adjustment.

6.3. PS2

The input data set contained 6 experimentally determined reaction rates, the input spectrum and its covariance matrix in 37 groups. The fact that all participants had difficulty with this set indicates that some serious inconsistency is present. Here also modifications of the input spectrum were made before starting the adjustment (by three participants). At present the origin of the inconsistency has not been identified completely, but information is available now that the spectrum covariance matrix was not correct. Participants tried to change the activity of the reaction rate for $^{56}\text{Fe}(n,\gamma)$, or the low energy part of the input spectrum; most participants suspected an irradiation in special covers, but none of these possibilities improved the situation completely.

6.4. TAN

The input data set contained 18 experimentally determined reaction rates and an input spectrum in 39 groups. The covariance matrix of this spectrum was based upon an estimation procedure.

The following observations can be made:

- More spectrum information in the thermal and intermediate neutron energy region is required.
- An inconsistency was observed in the input data by one participant, but the reason could not be traced. The reactions $^{45}\text{Sc}(n,\gamma)$, $^{235}\text{U}(n,f)$ and $^{238}\text{U}(n,f)$ showed large relative χ^2 -contributions in this solution.

6.5. RTN

The input data set contained 12 experimentally determined reaction rates and an input spectrum in 60 groups. The covariance matrix of

this spectrum (in 60 groups) was based upon estimates. Also this set showed an inconsistency. Large relative χ^2 -contributions were found for the reactions $^{197}\text{Au}(n,\gamma)$, $^{47}\text{Ti}(n,p)$ and $^{60}\text{Ni}(n,p)$.

The following observations can be made:

- The thermal reactions have been irradiated in a cadmium cover which fact was not communicated to the participants.
- Improved input spectrum information for the thermal and intermediate part of the neutron spectrum is required.

6.6. U35

The input data set contained 22 experimentally determined reaction rates and an input spectrum in 24 groups together with a covariance matrix in 24 groups. The covariance matrix has uncertainties which are so small that not really a modification of the spectrum could be expected. Therefore, the adjustment procedure has more the character of a test on consistency of the numerical data and on correctness of calculation procedures.

The following observations can be made:

- Several reactions have large cross-section uncertainties:
 $^{47}\text{Ti}(n,p)$, $^{60}\text{Ni}(n,2n)$ and $^{127}\text{I}(n,2n)$.
- One participant obtained "negative" variances in the calculations (SET 6).
- The group structure is inadequate for the calculation of $(n,2n)$ reactions.
- Also at the low energy side a finer group structure is needed.

6.7. CFR

The input data set contained 23 experimentally determined reaction rates and an input spectrum in 26 groups. Also in this case the quality of the spectrum covariance matrix was such that an adjustment of the spectrum could not really be expected.

The following observations can be made:

- The cross-section information of the reaction $^{47}\text{Ti}(n,p)$ is not correct.
- The $^{116}\text{In}(n,\gamma)^{116}\text{In}^{\text{m}}$ cross-section data are not readily available.
- Large relative χ^2 -contributions were found for the reaction

- $^{59}\text{Co}(n,\gamma)$. This is probably due to a too coarse input spectrum structure at the resonance region of the $^{59}\text{Co}(n,\gamma)$ cross-section.
- More input spectrum information is required in the resonance region.
 - The group structure of the spectrum is too coarse, which resulted also in difficulties for reactions with response above 6 MeV.

7. CONCLUSIONS

7.1. Input data sets

General

1. The actual situation with respect to consistency and quality of the input data is disappointing. Sometimes large inconsistencies in the input data set were found (PS1, PS2, CFR), detected e.g. by an unacceptable χ^2 -value or by discrepant reaction rates (see section 4.4). The participants had different actions for the solution of this problem. They changed the weight (variance) of some reaction rates in the calculations, deleted reactions from the adjustment, or modified the input spectrum.
2. In a late phase of the exercise it was communicated that in case of the spectrum PS1 all detectors were irradiated in a gadolinium cover. The total cross-section of the Gd was made available, but not all participants were in the position to perform the necessary corrections.

Spectrum and group structure

1. For all seven spectra (ANO, PS1, PS2, TAN, RTN, U35, CFR) a finer group structure in the low energy region, and for ANO, U35, CFR in the high energy region (above 3-6 MeV), would have been required to achieve a more adequate description of these parts of the spectra (see section 3.9). This finer group structure is necessary for a more accurate calculation of activation, fission and damage rates.

Spectrum covariances (see section 3.5)

1. The uncertainty of the input spectrum was very large for ANO, and very small for U35 and CFR. As a result, no real spectrum adjustment could be expected in the latter cases.
2. Correlation matrices based on reactor physics calculations were available for the spectra ANO, PS1, PS2, U35, CFR. In other cases "good estimates" or artificially created correlation matrices were used. As the input (and output) spectrum covariance matrix

has an important role in the uncertainty assessment of the damage parameters, the lack of realistic data may lead to an incorrect estimate of the corresponding standard deviations.

3. Identical input spectrum covariance matrices were given for the spectra PS1 and PS2. As these spectra represent different irradiation positions, the two correlation matrices can in principle not be identical. At the end of this REAL84 exercise improved matrices became available.
4. All input spectrum covariance matrices were found to be singular within computer accuracy (table 2).

Reaction rates and their uncertainties

1. Sometimes the number of available experimentally determined reaction rates was small and a typical thermal response was lacking (e.g. in case of ANO) (see section 3.4).
2. For many of the spectra only variances for the measured reaction rates were supplied. In these cases diagonal covariance matrices had to be used in the calculations.
3. In some cases (e.g. spectrum ANO and PS1) very large uncertainties for the measured reaction rates were found.

Cross-section data

1. In a number of cases clearly inadequate values for cross-sections and cross-section uncertainties derived from the most up-to-date version of ENDF/B-V and IRDF-85 libraries were found by several participants.

Also a number of reaction rates could not be applied in the exercise, due to absence of cross-section data (see sections 3.2 and 3.6).

7.2. Output of the exercise

General

1. In some cases the solutions were given in a group structure (e.g. 98, 100, 215) different from the input one. Sometimes a participant supplied for the same spectrum case more solutions, obtained by different adjustment codes and/or different energy group structures.
2. A large spread in the calculated input and output reaction rates can often be observed (PS1, PS2, CFR). This fact indicates the presence of inconsistencies in the input data set and/or reflects the effect of different data treatment and calculation procedures applied by the participants.

Calculation procedure

1. Most of the calculations were performed by spectrum adjustment codes based on the generalized least-squares procedure, except the two cases, in which a SAND type code - in one case combined with Monte-Carlo uncertainty analysis - was used. The latter method gave practically the same results as the least-squares ones (see section 4.1).
2. In many cases the participants used various procedures for the normalization on the input reaction rates. This fact resulted in different input spectra, which consequently led to deviating results (see section 4.5).

Integral (damage) parameters

The absolute values for integral parameters, which have been calculated by the various participants, show some spread.

The interlaboratory standard deviations is listed for some parameters in table 15a. Table 15b shows the average of the calculated uncertainties by the participants. A comparison of the data of tables 15a and b shows that the interlaboratory spread is not low with respect to the calculated uncertainties.

This means that the total uncertainty for the parameter of interest will be larger than the one predicted by the participants. It is evident that the interlaboratory spread has to be reduced by improving the input data and the adjustment process (comprising the extension of the number of activation and/or fission reactions and the improvement of the covariance data in the input data set.

7.3. Recommendations for adjusting neutron spectra

1. More attention should be given to elimination of inconsistencies in the input data set. In this respect one should try to include more "physics" in the information on the experiment and calculation procedures.
2. More effort should be spent to obtain good quality spectrum covariance matrices. In cases where no covariance matrix for the input neutron spectrum is available, one should preferably use an approximation from another similar type of reactor rather than an artificial band matrix.
3. In order to avoid systematic deviations in group cross-section values it is necessary to have the input neutron spectrum available in a more detailed group structure, specially for the lower and higher energy regions.
4. For the characterization of input and output data of neutron spectrum adjustment one should quote:
 - a) the measured (or calculated) values;
 - b) their variances;
 - c) the corresponding correlation matrices;
 - d) if possible, the numerical (i.e. effective) rank of the correlation matrix, and the way of defining it;
 - e) the calculation method of input spectrum and the spectrum covariance matrix.

In view of further calculations, it is recommended to communicate the correlation data in a precise form, and not rounded to only 2 or 3 digits, especially for ill-conditioned matrices.

5. In neutron spectrum adjustments one should distinguish between scaling and normalization. Scaling refers to the determination of

a rough spectrum conversion factor needed to arrive at comparable values of calculated and measured reaction rates. Normalization refers to the determination of a spectrum fine tuning factor (a factor near unity), needed to arrive at the best fit between calculated and measured reaction rates. The normalization is recommended to be determined with a least-squares method as indicated in [1].

6. In principle the uncertainty of the spectrum normalization factor should be incorporated in the input spectrum covariance matrix (and its associated correlation matrix) before starting the final adjustment procedure.
7. Adequate numerical procedures which take into account the relevant covariances should be used to describe the uncertainty propagation in damage parameter calculations.
8. For numerical reasons it is better in computer calculations to work with correlation matrices than with covariance matrices.
9. Basically, full-rank (positive definite) correlation matrices would be needed for the neutron spectrum adjustment by non-linear methods (involving matrix inversion) and for correct description of the uncertainty propagation. Moreover, it is also known that these matrices are not available at this moment; in the best cases positive semi-definite matrices are available in the required group structure. One should keep in mind that these data from the point of view of mathematical statistics are only approximations to the correct positive definite matrices and so they give only approximations of the expected values. For this reason further development in this field is required.

7.4. Recommendations to the IAEA

1. The IAEA Nuclear Data Section should prepare an updated version of the International Reactor Dosimetry File (IRDF-88), and should distribute this version within two years with a good documentation.
2. In order to be able to perform improved uncertainty assessment of integral parameters, one needs more accurate information than given in file 33 of IRDF-85 for a number of reactions.

3. The IAEA Nuclear Data Section, the existing working groups involved in the compilation of the ENDF, and all evaluators involved, are kindly requested to improve the scattering cross-section data and the cross-section variance and covariance data, especially for iron.
4. The IAEA should promote the preparation of a reference data set for neutron spectrum adjustment procedures, based on the experience obtained in the REAL-84 exercise, and comprising a modified and improved data set, preferably with the same spectrum cases as in REAL-84 (ACTION: REAL-88). The aim of such a reference data set is to provide a tool for testing neutron spectrum adjustment codes by means of an unambiguous test case. The most important modification of the REAL88 set with respect to the REAL84 input data set will be the improved consistency for each set. The reference data file should preferably comprise also important utility programs. Calculation results obtained by various laboratories for the reference file should be compiled. Tables with these data should be prepared for the reference set, showing the observed spread in results (comprising interlaboratory variation and range of reported coefficients of variation) which is observed when this well defined reference data set was treated without changes by different laboratories, with different adjustment codes and different computers.
IAEA should then distribute the resulting reference data set upon request to all experienced or new-coming laboratories interested in neutron spectrum adjustment procedures.
5. IAEA should promote the establishment and the distribution of a simple reactor physics code which neutron metrologists can use to calculate neutron self-shielding factors and cover attenuation factors for foil covers, required in irradiation experiments where covers and relatively thick activation detectors (foils and wires) are used.

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Table 1. Technical details for the input information and references.

input data	measured reaction rates	covariances for measured reaction rates	calculated input spectrum	covariances for calculated input spectrum
ANO	6 reaction rates; no subcadmium responses [5]	available [6]	55 groups [7]	16 groups [7]
PS1	10 reaction rates [8]	only variances [8]	37 groups calculated [8]	37 groups calculated [8]
PS2	6 reaction rates [8]	only variances [8]	37 groups calculated [8]	37 groups calculated [8]
RTN	12 reaction rates [9]	available [9]	60 groups [9]	good estimates 60 groups [9]
TAN	18 reaction rates [9]	available [9]	39 groups [9]	good estimates 39 groups [9]
U35	22 reaction rates [10]	only variances [10]	24 groups [11]	24 groups [11]
CFR	23 reaction rates [10]	only variances [10]	26 groups [12]	26 groups [12]

Table 2. Characteristic data of correlation matrices.

Meaning of rows:

- 0) spectrum
- 1) number of groups
- 2) number of positive eigenvalues
- 3) number of zero eigenvalues
- 4) number of negative eigenvalues
- 5) effective rank [1] using single precision arithmetic (4 bytes)
- 6) effective rank [1] using double precision arithmetic (8 bytes)
- 7) number of eigenvalues greater than 1
- 8) number of eigenvalues to 98 per cent of the trace
- 9) logarithm of the condition number.

.. cannot be interpreted

Table 2a. ANO.

0)	INPUT	SET1	SET5	SET6	SET8	SET8A	SET9	SET12
1)	16	55	55	55	55	16	16	16
2)	16	42	36	38	36	16	15	16
3)	0	1	0	9	0	0	0	0
4)	0	12	19	8	19	0	1	0
5)	16	16	16	19	46	16	16	16
6)	16	16	30	19	55	16	16	16
7)	3	4	5	6	6	4	3	4
8)	9	8	13	13	13	13	7	14
9)	2.7	..	19.6	..	6.8	1.7	5.2	1.6

Table 2b. PS1.

0)	INPUT	SET5	SET6	SET12A
1)	37	37	36	37
2)	37	37	36	37
3)	0	0	0	0
4)	0	0	0	0
5)	37	37	36	37
6)	37	37	36	37
7)	4	9	9	5
8)	14	25	24	20
9)	3.3	2.5	4.5	2.9

Table 2c. PS2.

0)	INPUT	SET5	SET6	SET9	SET12A
1)	37	37	37	37	37
2)	37	37	37	33	37
3)	0	0	0	0	0
4)	0	0	0	4	0
5)	37	37	37	34	37
6)	37	37	37	37	37
7)	4	7	8	6	7
8)	14	23	24	12	23
9)	3.3	2.8	3.5	8.4	2.7

Table 2d. TAN.

0)	INPUT*	SET6
1)	39*	39
2)	25*	27
3)	0*	0
4)	14*	12
5)	39*	39
6)	39*	39
7)	5*	6
8)	6*	7
9)	5.9*	4.9

* Artificial band matrix, no physical meaning.

Table 2e. RTN.

0)	INPUT*	SET6	SET7
1)	60*	60	60
2)	40*	46	40
3)	0*	0	0
4)	20*	14	20
5)	60*	58	58
6)	60*	60	60
7)	10*	10	10
8)	12*	13	13
9)	5.9*	5.6	5.7

* Artificial band matrix, no physical meaning.

Table 2f. U35.

0)	INPUT	SET5	SET6	SET7	SET8	SET9	INPUT*
1)	24	24	24	24	24	24	24*
2)	13	14	13	14	16	18	12*
3)	0	0	0	0	0	0	0*
4)	11	10	11	10	8	6	12*
5)	22	24	22	23	23	24	12*
6)	24	24	24	24	24	24	23*
7)	2	2	2	2	2	2	..*
8)	2	2	2	2	2	7	2*
9)	6.4	5.2	5.6	5.4	5.3	4.1	21.3*

* Data of the covariance matrix (for comparison only).

Table 2g. CFR.

0)	INPUT	SET5	SET6	SET12
1)	26	26	26	26
2)	20	21	21	21
3)	0	0	0	0
4)	6	5	5	5
5)	26	26	26	26
6)	26	26	26	26
7)	6	6	6	6
8)	6	10	12	10
9)	3.7	3.4	3.6	3.4

Table 3. Role of cross-section uncertainties in reaction rate calculations.

reaction	spectrum									
	ANO	PS1	PS2	TAN	RTN	U35	CFR	ϕ_{th}	$\phi_{1/E}$	ϕ_{fiss}
${}^6\text{Li}(n,\alpha)$							0	0	0	0
${}^{10}\text{B}(n,\alpha)$							0	0	0	-
${}^{27}\text{Al}(n,p)$						-	-			-
${}^{27}\text{Al}(n,\alpha)$				0	0	-	-			-
${}^{45}\text{Sc}(n,\gamma)$		0	0	-	0		0	0	0	0
${}^{46}\text{Ti}(n,p)$	--	--	--	--	--	--	--			--
${}^{47}\text{Ti}(n,p)$				--	--	--	--		--	--
${}^{48}\text{Ti}(n,p)$				--	--	--	--			--
${}^{54}\text{Fe}(n,p)$	0	0	0	0	-	0	0		-	0
${}^{55}\text{Mn}(n,2n)$						--				--
${}^{56}\text{Fe}(n,p)$				0		0				0
${}^{58}\text{Fe}(n,\gamma)$		--	--				--	-	--	--
${}^{58}\text{Ni}(n,p)$	-	-	-	-	--	-	-		-	-
${}^{58}\text{Ni}(n,2n)$				--	--	--				--
${}^{59}\text{Co}(n,\gamma)$		0	0	-	0		0	0	0	0
${}^{59}\text{Co}(n,\alpha)$				0		0				0
${}^{59}\text{Co}(n,2n)$				-	-					--
${}^{60}\text{Ni}(n,p)$				-	-					-
${}^{63}\text{Cu}(n,\gamma)$						--	-	0	0	--
${}^{63}\text{Cu}(n,\alpha)$	-	-				-				-
${}^{115}\text{In}(n,\gamma)$						0	0	-	-	0
${}^{115}\text{In}(n,n')$				--		--	--		--	--
${}^{127}\text{I}(n,2n)$						--				--
${}^{197}\text{Au}(n,\gamma)$				--	0	-	0	0	0	-
${}^{232}\text{Th}(n,\gamma)$							--	-	--	--
${}^{232}\text{Th}(n,f)$						-	-		-	-
${}^{235}\text{U}(n,f)$		0		0		0	0	0	0	0
${}^{237}\text{Np}(n,f)$	-	-				-	-	--	--	-
${}^{238}\text{U}(n,\gamma)$				--			0	0	0	0
${}^{238}\text{U}(n,f)$	0	0		0		0	0	--	-	0
${}^{239}\text{Pu}(n,f)$						0	0	0	-	0

0 : uncertainty in calculated reaction rate: 0- 5%
 - : uncertainty in calculated reaction rate: 5-10%
 --: uncertainty in calculated reaction rate: > 10%

Table 4. Survey of participating laboratories : supplied solutions

Laboratory code	Participant	Ident of solution	Adjustment code	Spectrum
NRMI	U. Ueda, M. Nakazawa, A. Sekiguchi	SET 1	NEUPAC-JLOG	ANO
ORNL	R.E. Maerker	SET 2	LEPRICON	ANO*
ANL	L.R. Greenwood	SET 3	STAY'SL	ANO, PS1, PS2, TAN*, RTN*, U35, CFR
IJS	M.Najzer, I. Remec	SET 4	STAY'SL	ANO
KFKI	J. Végh	SET 5	STAY'SL	ANO, PS1, PS2, U35, CFR
ECN	H.J. Nolthenius	SET 6	STAYNL	ANO, PS1, PS2, TAN, RTN, U35, CFR
PTB	M. Matzke, W. Mannhart	SET 7	STAY'SL	RTN, U35
BME	É.M. Zsolnay, E.J. Szondi	SET 8 SET 9	STAYNL SANDBP	ANO, U35 ANO, PS2, U35
IPM	A. Hrabovcova	SET 10	SANDBP	ANO, TAN, RTN
ORNL	F.W. Stallmann	SET 11	LSL-M2	PS1, PS2
ZFK	B. Böhmer	SET 12	STAYS'L-ZFK	ANO, PS1, PS2, CFR
NRI+SW	B. Osmera, J. Hadek, F. Vychytíl	SET 13	STAYS'L-SK	PS2

* More than one solution

Table 5a. Calculated reaction rates for input spectrum of ANO.

REACTION	MEASURED	NEUPAC- JLOG	LEPRICON	LEPRICON (1)	STAY'SL	STAY'SL + 2 MOD	STAY'SL
CU63A	1.900E-19	R84 SET 1 1.987E-19	R84 SET 2 1.470E-19	R84 SET 2A 1.470E-19	R84 SET 3 1.704E-19	R84 SET 4 1.724E-19	R84 SET 5 1.800E-19
TI46P	2.350E-18	2.346E-18	1.970E-18	1.970E-18	2.370E-18	2.039E-18	2.110E-18
NI58P	1.730E-17	1.648E-17	1.450E-17	1.450E-17	1.697E-17	1.523E-17	1.570E-17
FE54P	1.260E-17	1.204E-17	1.050E-17	1.050E-17	1.240E-17	1.044E-17	1.070E-17
U238F	7.420E-17	6.973E-17	5.810E-17	5.810E-17	7.248E-17	6.043E-17	6.220E-17
NP237F	1.070E-15	1.213E-15	1.040E-15	1.040E-15	1.219E-15	1.043E-15	1.070E-15
REACTION	STAYNL	STAYNL	SANDBP	SAND-MX	STAYSL-ZFK		
	STAY'SL MOD						
CU63A	R84 SET 6 1.853E-19	R84 SET 8 1.907E-19	R84 SET 8A 1.913E-19	R84 SET 9 1.990E-19	R84 SET 10 3.310E-19	R84 SET 12 1.971E-19	
TI46P	2.180E-18	2.245E-18	2.250E-18	2.357E-18	3.510E-18	2.320E-18	
NI58P	1.616E-17	1.665E-17	1.666E-17	1.705E-17	1.680E-17	1.728E-17	
FE54P	1.109E-17	1.142E-17	1.144E-17	1.160E-17	1.320E-17	1.180E-17	
U238F	6.424E-17	6.607E-17	6.589E-17	6.947E-17	3.610E-17	6.822E-17	
NP237F	1.108E-15	1.140E-15	1.135E-15	1.218E-15	2.750E-16	1.176E-15	

Table 5b. Calculated reaction rates for input spectrum of U35.

REACTION	MEASURED	STAY'SL	STAY'SL	STAY'SL MOD	STAYS�	STAYNL	SANDBP
		R84 SET 3	R84 SET 5	R84 SET 6	R84 SET 7	R84 SET 8	R84 SET 9
AL27P	3.650E-10	4.323E-10	4.250E-10	4.191E-10	4.265E-10	4.167E-10	4.222E-10
AL27A	7.050E-11	7.929E-11	7.140E-11	7.055E-11	7.218E-11	7.118E-11	7.213E-11
TI46P	1.180E-09	1.134E-09	1.110E-09	1.099E-09	1.119E-09	1.093E-09	1.107E-09
TI47P	1.900E-09	2.188E-09	2.230E-09	2.200E-09	2.243E-09	2.188E-09	2.217E-09
TI48P	3.000E-11	3.075E-11	2.800E-11	2.783E-11	2.829E-11	2.764E-11	2.833E-11
FE54P	7.810E-09	7.928E-09	8.040E-09	7.937E-09	8.089E-09	7.892E-09	7.995E-09
MN552	2.440E-11	2.454E-11	2.070E-11	2.584E-11	2.094E-11	2.382E-11	2.414E-11
FE56P	1.025E-10	1.104E-10	1.030E-10	1.021E-10	1.039E-10	1.020E-10	1.033E-10
NI582	5.770E-13	3.827E-13	2.730E-13	6.293E-13	.000E+00	4.664E-13	4.726E-13
NI58P	1.085E-08	1.026E-08	1.040E-08	1.030E-08	1.050E-08	1.024E-08	1.038E-08
CO59A	1.430E-11	1.631E-11	1.490E-11	1.476E-11	1.503E-11	1.482E-11	1.502E-11
CU63A	5.000E-11	5.449E-11	5.550E-11	5.482E-11	5.592E-11	5.487E-11	5.560E-11
CU63G	9.300E-10	9.375E-10	9.800E-10	9.667E-10	9.859E-10	9.627E-10	9.755E-10
IN115N	1.890E-08	1.721E-08	1.780E-08	1.754E-08	1.790E-08	1.747E-08	1.770E-08
IN115G	1.345E-08	1.182E-08	1.350E-08	1.546E-08	1.577E-08	1.540E-08	1.560E-08
I1272	1.050E-10	1.446E-10	1.210E-10	1.281E-10	1.238E-10	1.289E-10	1.306E-10
AU197G	8.350E-09	7.426E-09	7.780E-09	7.680E-09	7.827E-09	7.651E-09	7.752E-09
TH232F	8.100E-09	7.268E-09	7.450E-09	7.357E-09	7.500E-09	7.325E-09	7.421E-09
U235F	1.203E-07	1.180E-07	1.230E-07	1.211E-07	1.235E-07	1.206E-07	1.222E-07
U238F	3.050E-08	2.945E-08	3.030E-08	2.993E-08	3.051E-08	2.979E-08	3.018E-08
NP237F	1.312E-07	1.289E-07	1.340E-07	1.322E-07	1.346E-07	1.314E-07	1.331E-07
PU239F	1.811E-07	1.710E-07	1.780E-07	1.755E-07	1.790E-07	1.747E-07	1.770E-07

Table 6. χ^2 -values for STAY-SL type solutions.

spectrum	χ^2		number of solutions
	minimum	maximum	
ANO	1.59×10^{-1}	3.75×10^{-1}	6
PS1	1.00	1.63	3
PS2	4.40×10^{-1}	17.4	4
TAN	4.77×10^{-1}	5.62×10^{-1}	2
RTN	4.72×10^{-1}	3.39×10^{-1}	5
U35	5.61×10^{-1}	1.29	5
CFR	1.59	7.07	4

Table 7. Average evaluators' normalization and spread of input and output spectra (calculated from the reaction rates).

spectrum	input		output		number of solutions
	average	s.d. (in %)	average	s.d. (in %)	
ANO	0.944	6.7	0.988	0.9	12
PS1	1.016	10.5	1.016	7.2	5
PS2	1.347	68.1	0.992	5.0	7
TAN	1.018	4.3	0.989	1.1	4
RTN (8.76	218.3	0.952	2.7	6
	0.952	3.4			5
U35	1.012	1.4	0.999	2.3	6
CFR	1.018	3.7	0.982	3.0	4

Table 8a. Calculated reaction ratios for output for ANO.

REACTION	C/E RATIOS FOR OUTPUT											
	R84 SET 1	R84 SET 2	R84 SET 2A	R84 SET 3	R84 SET 4	R84 SET 5	R84 SET 6	R84 SET 8	R84 SET 8A	R84 SET 9	R84 SET 10	R84 SET 12
CU63A	1.02	.96	.89	.96	1.00	1.01	1.01	1.01	1.01	1.05	1.00	1.02
TI46P	1.01	1.02	1.07	1.06	1.00	1.00	1.00	1.00	1.01	1.01	1.03	1.00
NI58P	.98	.99	1.06	1.00	1.01	1.01	1.02	1.02	1.00	1.00	.99	1.02
FE54P	.99	.99	1.06	1.00	.96	.96	.97	.97	.94	.94	.95	.97
U238F	.95	.91	.90	.97	.92	.93	.93	.93	.95	.95	.90	.93
NP237F	1.11	1.00	1.03	1.08	1.05	1.07	1.07	1.07	1.06	1.06	1.06	1.08

C/E RATIOS FOR OUTPUT

Table 8b. Calculated reaction ratios for output for PSI.

REACTION	C/E RATIOS FOR OUTPUT											
	R84 SET 3	R84 SET 5	R84 SET 6	R84 SET 11	R84 SET 12							
U235F	1.07	1.06	1.17	1.04	1.45							
CO59G	.96	.95	.99	1.00	.75							
SC45G	.97	.97	.95	.99	.97							
FE58G	1.30	1.21	1.24	1.01	1.63							
U238F	.91	.95	.95	.95	.95							
NP237F	.88	.95	.96	.97	.98							
NI58P	.95	.97	.96	.98	.96							
FE54P	1.04	1.05	1.03	1.04	1.03							
TI46P	.95	.94	.92	.96	.92							
CU63A	.97	1.02	1.01	1.00	1.00							

Table 9a. Normalized ratios for input for ANO

REACTION	R84 SET 1	R84 SET 2	R84 SET 2A	R84 SET 3	R84 SET 4	R84 SET 5
CU63A	-4.13	7.87	7.87	10.11	-3.24	-4.48
TI46P	.60	.17	.17	-1.08	1.27	.97
NI58P	5.15	.19	.19	1.69	-.17	-.09
FE54P	4.85	.76	.76	1.36	5.72	6.34
U238F	6.42	6.75	6.75	2.10	7.33	7.55
NP237F	-12.88	-15.75	-15.75	-14.18	-10.91	-10.29
NORMALIZATION	1.004E+00	8.397E-01	8.397E-01	9.977E-01	8.789E-01	9.067E-01

REACTION	R84 SET 6	R84 SET 8	R84 SET 8A	R84 SET 9	R84 SET 10	R84 SET 12
CU63A	-4.15	-4.12	-4.44	-4.20	-74.27	-4.11
TI46P	.93	.89	.93	.22	-49.41	.92
NI58P	.25	.16	.10	1.95	2.86	-.24
FE54P	6.01	5.97	5.82	8.41	-4.80	6.01
U238F	7.54	7.63	7.88	6.86	51.33	7.73
NP237F	-10.58	-10.53	-10.04	-13.24	74.29	-10.30
NORMALIZATION	9.364E-01	9.639E-01	9.640E-01	1.005E+00	9.997E-01	9.964E-01

Table 9b. Normalized ratios for input for PS1.

REACTION	R84 SET 3	R84 SET 5	R84 SET 6	R84 SET 11	R84 SET 12
U235F	-12.59	-4.74	-12.01	-50.91	-20.71
CO59G	-13.03	-4.94	-1.86	-3.64	49.02
SC45G	4.71	9.31	17.91	-57.15	11.20
FE58G	-47.04	-29.23	-23.39	-45.41	-12.02
U238F	13.62	7.07	5.33	27.60	-2.44
NP237F	14.97	6.29	4.69	26.80	-3.80
NI58P	11.31	5.95	4.14	27.35	-3.47
FE54P	3.15	-.74	-2.76	21.11	-10.94
TI46P	13.00	9.48	8.11	29.65	1.02
CU63A	11.90	1.55	-.16	24.58	-7.85
NORMALIZATION	9.447E-01	9.534E-01	1.014E+00	1.200E+00	9.669E-01

Table 10a. Normalized ratios for output for ANO.

REACTION	R84 SET 1	R84 SET 2	R84 SET 2A	R84 SET 3	R84 SET 4	R84 SET 5
CU63A	-1.00	1.79	10.60	5.17	-1.57	-1.40
TI46P	-.38	-4.13	-7.15	-4.65	-.62	.27
NI58P	2.88	-1.37	-5.70	1.45	-2.08	-1.37
FE54P	2.27	-1.15	-5.47	.72	3.00	4.05
U238F	5.76	6.83	10.45	4.43	7.26	6.92
NP237F	-9.53	-1.96	-2.72	-7.12	-6.00	-8.48
NORMALIZATION	1.009E+00	9.807E-01	1.001E+00	1.011E+00	9.892E-01	9.951E-01

REACTION	R84 SET 6	R84 SET 8	R84 SET 8A	R84 SET 9	R84 SET 10	R84 SET 12
CU63A	-1.51	-1.42	-1.53	-4.39	-1.25	-1.26
TI46P	-.36	-.27	-.36	-1.22	-3.84	.00
NI58P	-1.80	-1.73	-1.78	.07	-.67	-1.99
FE54P	3.42	3.52	3.39	5.73	3.57	3.66
U238F	7.04	7.07	7.21	5.23	9.12	7.06
NP237F	-6.79	-7.16	-6.93	-5.41	-6.93	-7.48
NORMALIZATION	9.960E-01	9.995E-01	9.990E-01	1.002E+00	9.876E-01	1.003E+00

Table 10b. Normalized ratios for output for PS1.

REACTION	R84 SET 3	R84 SET 5	R84 SET 6	R84 SET 11	R84 SET 12
U235F	-7.03	-4.85	-15.29	-4.61	-36.29
CO59G	4.17	5.21	3.04	-.23	29.83
SC45G	3.39	3.74	6.62	.51	8.49
FE58G	-29.86	-20.06	-21.85	-2.01	-53.04
U238F	8.47	5.19	6.56	4.31	10.44
NP237F	11.63	6.00	5.91	2.10	7.82
NI58P	4.83	3.31	5.51	1.46	9.72
FE54P	-4.17	-3.90	-1.23	-4.34	3.29
TI46P	5.22	6.62	9.45	3.41	13.57
CU63A	3.36	-1.26	1.28	-.59	5.72
NORMALIZATION	9.992E-01	1.007E+00	1.019E+00	9.933E-01	1.066E+00

Table 11. Contribution of non-linear terms.

spectrum	reaction	relative contribution (in per cent)		influence in weight	
		in	out	input	output
ANO	CU63A	5.1	4.8	1.003	1.002
ANO	TI46P	11.0	6.4	1.012	1.004
ANO	NI58P	5.6	2.9	1.003	1.001
ANO	FE54P	3.3	3.3	1.001	1.001
ANO	U238F	2.5	2.9	1.001	1.001
ANO	NP237F	8.5	6.6	1.007	1.004
PS1	U235F	2.2	2.4	1.000	1.001
PS1	C059G	0.8	0.8	1.000	1.000
PS1	SC45G	1.1	1.2	1.000	1.000
PS1	FE58G	15.5	4.9	1.025	1.002
PS1	U238F	2.3	2.5	1.001	1.001
PS1	NP237F	9.4	4.9	1.009	1.002
PS1	NI58P	6.0	3.6	1.004	1.001
PS1	FE54P	3.5	2.8	1.001	1.001
PS1	TI46P	10.1	3.7	1.010	1.001
PS1	CU63A	5.1	3.7	1.003	1.001
PS2	C059G	0.8	0.9	1.000	1.000
PS2	SC45G	1.0	2.1	1.000	1.000
PS2	FE58G	11.0	7.6	1.012	1.006
PS2	NI58P	5.8	3.9	1.003	1.002
PS2	FE54P	3.4	2.8	1.001	1.001
PS2	TI46P	10.1	4.8	1.010	1.002
TAN	AL27A	4.4	2.3	1.002	1.001
TAN	AU197G	13.2	5.2	1.018	1.003
TAN	NI58P	5.4	2.5	1.003	1.001
TAN	NI582	8.9	4.4	1.008	1.002
TAN	NI60P	6.2	2.6	1.004	1.001
TAN	TI46P	10.0	2.2	1.010	1.000
TAN	TI47P	9.0	2.2	1.008	1.000
TAN	TI48P	9.0	2.7	1.008	1.001
TAN	SC45G	7.4	4.7	1.005	1.002
TAN	FE56P	3.7	1.9	1.001	1.000
TAN	C059G	7.2	4.2	1.005	1.002
TAN	C059A	4.0	2.3	1.002	1.001
TAN	FE54P	3.2	2.1	1.001	1.000
TAN	C0592	7.3	3.1	1.005	1.001
TAN	IN115N	9.6	3.0	1.009	1.001
TAN	U235F	2.8	2.1	1.001	1.000
TAN	U238F	2.0	1.9	1.000	1.000
TAN	U238G	8.9	4.8	1.008	1.002
RTN	SC45G	0.9	0.9	1.000	1.000
RTN	C059G	0.7	0.8	1.000	1.000
RTN	AU197G	3.0	2.0	1.001	1.000
RTN	TI46P	8.1	3.4	1.007	1.001
RTN	TI47P	7.9	3.3	1.006	1.001
RTN	TI48P	7.8	3.3	1.006	1.001
RTN	FE54P	5.4	3.1	1.003	1.001
RTN	NI58P	8.2	3.3	1.007	1.001
RTN	NI60P	6.1	3.2	1.004	1.001

Table 11 (continued).

spectrum	reaction	relative contribution (in per cent)		influence in weight	
		in	out	input	output
RTN	AL27A	3.4	2.4	1.001	1.001
RTN	C0592	4.9	3.0	1.002	1.001
RTN	NI582	7.4	3.3	1.006	1.001
U35	AL27P	3.9	1.8	1.002	1.000
U35	AL27A	4.6	2.5	1.002	1.001
U35	TI46P	5.2	1.9	1.003	1.000
U35	TI47P	3.1	1.1	1.001	1.000
U35	TI48P	6.6	2.8	1.004	1.001
U35	FE54P	2.3	1.1	1.001	1.000
U35	MN552	8.2	4.2	1.007	1.002
U35	FE56P	3.7	2.1	1.001	1.000
U35	NI582	8.6	4.3	1.008	1.002
U35	NI58P	2.8	1.2	1.001	1.000
U35	C059A	3.8	2.3	1.001	1.001
U35	CU63A	4.2	2.2	1.002	1.000
U35	CU63G	1.1	0.4	1.000	1.000
U35	IN115N	1.5	0.6	1.000	1.000
U35	IN115G	1.1	0.5	1.000	1.000
U35	I1272	10.0	4.1	1.010	1.002
U35	AU197G	0.7	0.2	1.000	1.000
U35	TH232F	2.3	1.0	1.001	1.000
U35	U235F	0.0	0.0	1.000	1.000
U35	U238F	1.4	0.5	1.000	1.000
U35	NP237F	0.7	0.3	1.000	1.000
U35	PU239F	1.0	0.0	1.000	1.000
CFR	LI6A	2.0	1.3	1.000	1.000
CFR	B10A	2.0	0.8	1.000	1.000
CFR	SC45G	2.2	2.0	1.001	1.000
CFR	FE58G	3.4	2.5	1.001	1.001
CFR	C059G	1.2	1.1	1.000	1.000
CFR	CU63G	1.5	1.0	1.000	1.000
CFR	IN115G	2.8	2.1	1.001	1.000
CFR	AU197G	2.7	2.2	1.001	1.000
CFR	TH232G	2.0	0.9	1.000	1.000
CFR	U238G	2.0	1.3	1.000	1.000
CFR	U235F	2.5	1.5	1.001	1.000
CFR	PU239F	2.5	1.9	1.001	1.000
CFR	NP237F	3.2	1.1	1.001	1.000
CFR	TH232F	4.2	2.0	1.002	1.000
CFR	U238F	2.0	1.7	1.000	1.000
CFR	IN115N	5.8	1.9	1.003	1.000
CFR	NI58P	5.2	2.1	1.003	1.000
CFR	FE54P	3.3	1.9	1.001	1.000
CFR	TI48P	6.8	3.7	1.005	1.001
CFR	TI47P	6.5	2.0	1.004	1.000
CFR	TI46P	6.9	2.2	1.005	1.000
CFR	AL27P	4.9	2.4	1.002	1.001
CFR	AL27A	4.6	2.8	1.002	1.001

Table 12. Uncertainty values for R_{dpa} steel.

The values are calculated by the evaluators, except the ones indicated with *. These are the averages of the participants' output values.

spectrum	uncertainty (in %)						
	before adjustment			after adjustment			
	total	ϕ contr.	σ contr.	total*	total	ϕ contr.	σ contr.
ANO	19.8	18.4	7.3	12.1 ⁺	11.6	9.0	7.3
PS1	14.9	12.9	7.4	9.8 ⁺	8.9	5.0	7.4
PS2	14.7	12.7	7.4	11.3 ⁺	9.4	5.9	7.3
TAN	19.0	16.9	8.7	8.7	1.8	8.5	8.5
RTN	14.1	10.0	10.0	10.6	10.6	3.5	10.0
U35	10.9	1.40	10.8	8.5	7.2	0.5	7.2
CFR	7.9	3.11	7.2	8.2	7.2	0.8	7.2

⁺ very large spread in participants' data.

Table 13. Uncertainty in spectrum characteristic integral data.

The values are calculated by the evaluators, except the ones indicated with *. These are the averages of the participants' output values.

spectrum	uncertainty (in %)								
	before adjustment			after adjustment					
	ϕ tot	ϕ >.1MeV	ϕ >1MeV	ϕ tot*	ϕ tot	ϕ >.1MeV*	ϕ >.1MeV	ϕ >1MeV*	ϕ >1MeV
ANO	20.5	18.4	20.8	13.3	13.1	10.6	10.3	8.8	8.8
PS1	36.0	12.2	13.6	---	5.4	6.1	5.9	5.5 ⁺	5.2
PS2	26.5	12.1	13.5	11.8 ⁺	6.5	9.5 ⁺	6.4	7.3 ⁺	5.9
TAN	16.3	16.3	16.3	---	2.3	---	2.3	---	2.3
RTN	9.7	9.9	10.0	3.3	3.4	3.3	3.4	3.4	3.5
U35	0	0.01	1.1	0.3	---	0.3	---	0.6	0.4
CFR	0.1	0.7	6.1	0.1	0.1	0.5	0.5	2.0	1.8

⁺ very large spread (20-70%) in participants' data.

Table 14. Sensitivity analysis of damage parameters.
(Part of solution of SET 1).

reaction	material	variance contributions			
		VC1	VC2	VC3	VC4
DPA	ST	13.4	8.7	27.9	50.0
	FE	16.4	10.5	32.9	40.2
	CR	8.8	5.7	18.5	67.0
	NI	13.2	9.5	33.3	44.0
HE	ST	6.2	2.1	1.1	90.6
	FE	20.3	9.5	7.2	63.0
	CR	9.7	5.2	5.9	79.2
	NI	16.3	3.9	3.2	76.6
H	ST	7.2	1.1	0.9	90.8
	FE	23.0	4.4	2.8	69.8
	CR	8.2	2.2	1.4	88.4
	NI	20.2	2.7	3.2	73.9

VC1: Contribution of reaction rate uncertainties to the variance of the DPA value (in per cent).

VC2: Contribution of reaction cross-section uncertainties to the variance of the DPA value (in per cent).

VC3: Contribution of output spectrum uncertainties to the variance of the DPA value (in per cent).

VC4: Contribution of DPA cross-section uncertainties to the variance of the DPA value (in per cent).

The sum of the four contributions is 100 per cent.

Table 15a. Interlaboratory standard deviation of some output parameters.
The number of solutions is indicated within brackets.
The standard deviation is given in per cent.

parameter	ANO	PS1	PS2	TAN	RTN	U35	CFR
♦>.1MeV	3.2 (11)	4.6 (5)	17. (4)	8.5 (4)	4.5 (6)	1.9 (6)	4.6 (4)
♦>1.MeV	6.2 (12)	3.8 (5)	13. (7)	7.9 (4)	4.6 (6)	2.2 (6)	6.3 (4)
R _{dpa} (Fe)	3.6 (11)	2.7 (4)	16. (6)	--- (1)	1.5 (2)	2.4 (6)	3.4 (4)
R _{dpa} (st)	3.1 (9)	3.1 (4)	16. (5)	--- (1)	8.0 (2)	2.3 (6)	3.4 (4)

Table 15b. Average predicted uncertainty value (and their spread, in per cent).

parameter	ANO	PS1	PS2	TAN	RTN	U35	CFR
♦>.1MeV	10.4 6.8	6.1 2.8	9.1 59.	2.3 3.1	3.8 15.	.4 15.	.5 14.
♦>1.MeV	8.6 10	5.4 4.7	7.3 42.	2.5 7.6	3.9 15.	.6 15.	2.0 13.
R _{dpa} (Fe)	11.2 15.	9.6 13.	9.7 29.	8.5 ---	10.5 .9	9.1 12.	8.9 21.
R _{dpa} (st)	10.6 21.	3.1 27.	9.4 25.	--- ---	8.5 0.	7.4 21.	7.1 37.

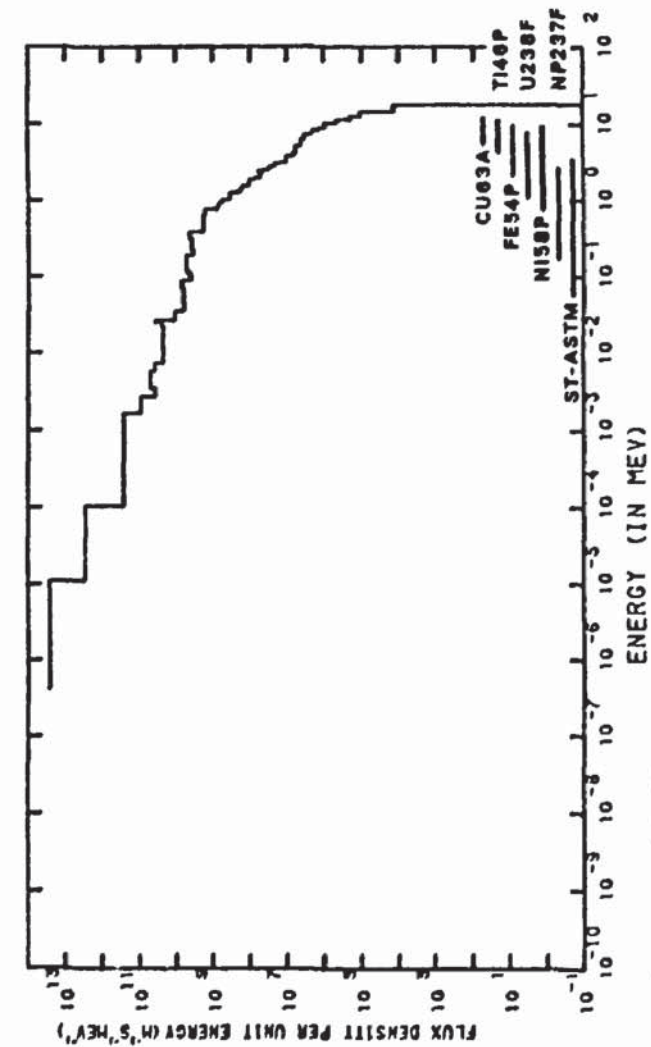


FIG. 1a. ANO SPECTRUM REAL84 EXERCISE

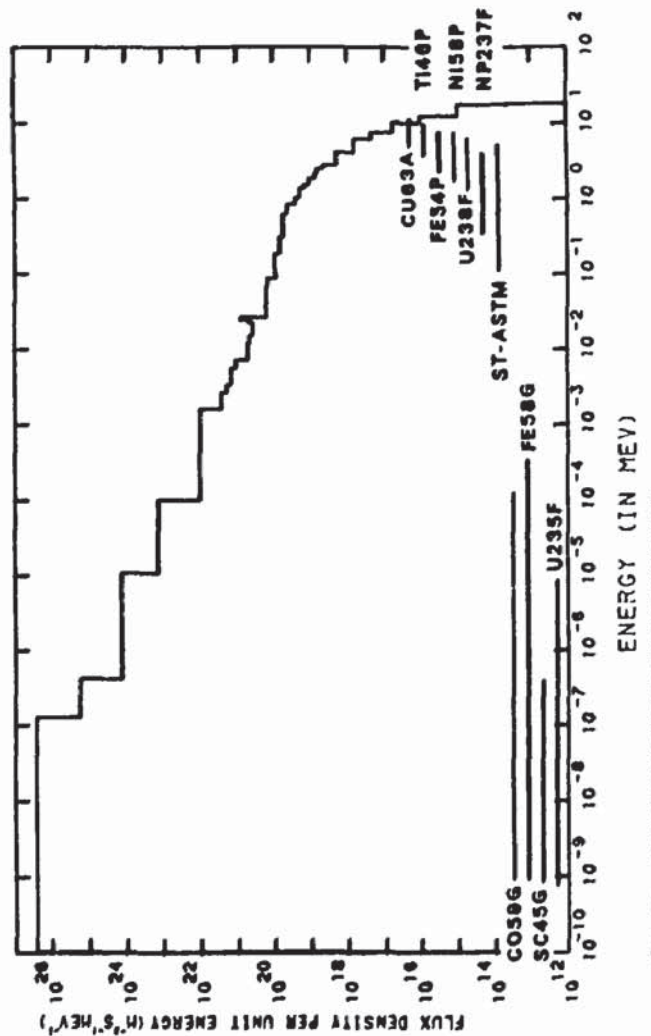


FIG. 1c. PS1 SPECTRUM REAL84 EXERCISE

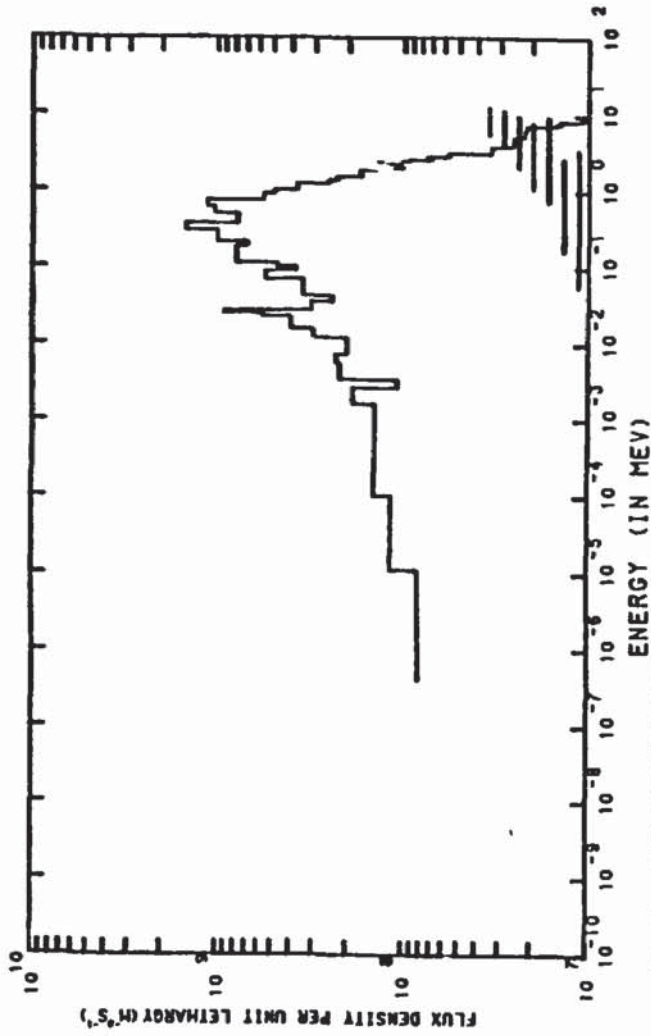


FIG. 1b. ANO SPECTRUM REAL84 EXERCISE

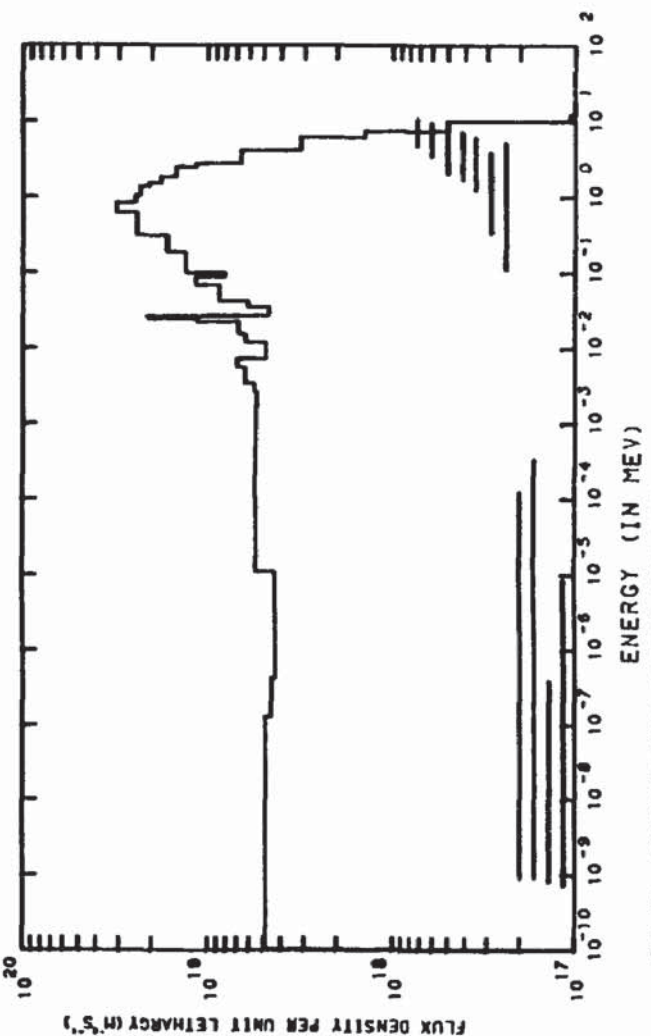


FIG. 1d. PS1 SPECTRUM REAL84 EXERCISE

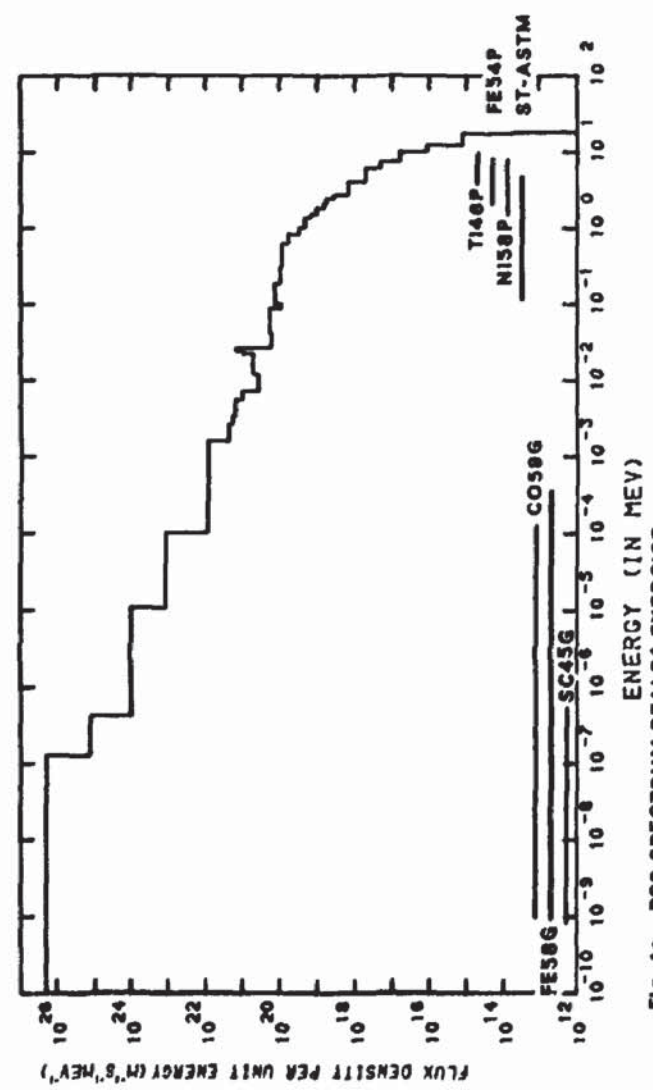


Fig. 10. PS2 SPECTRUM REAL84 EXERCISE

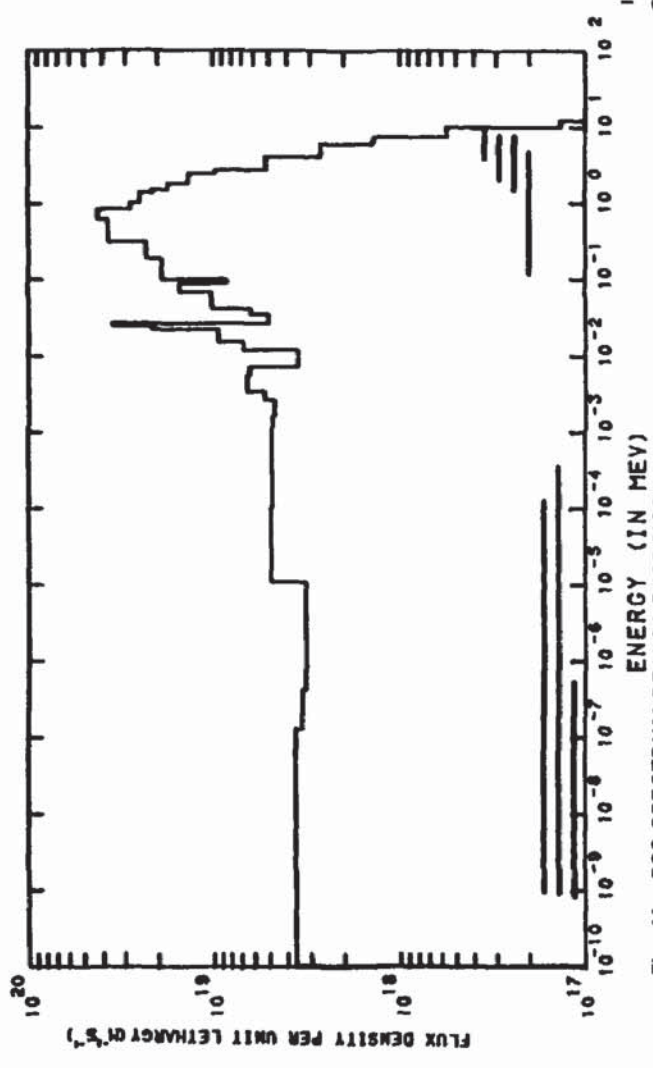


Fig. 11. PS2 SPECTRUM REAL84 EXERCISE

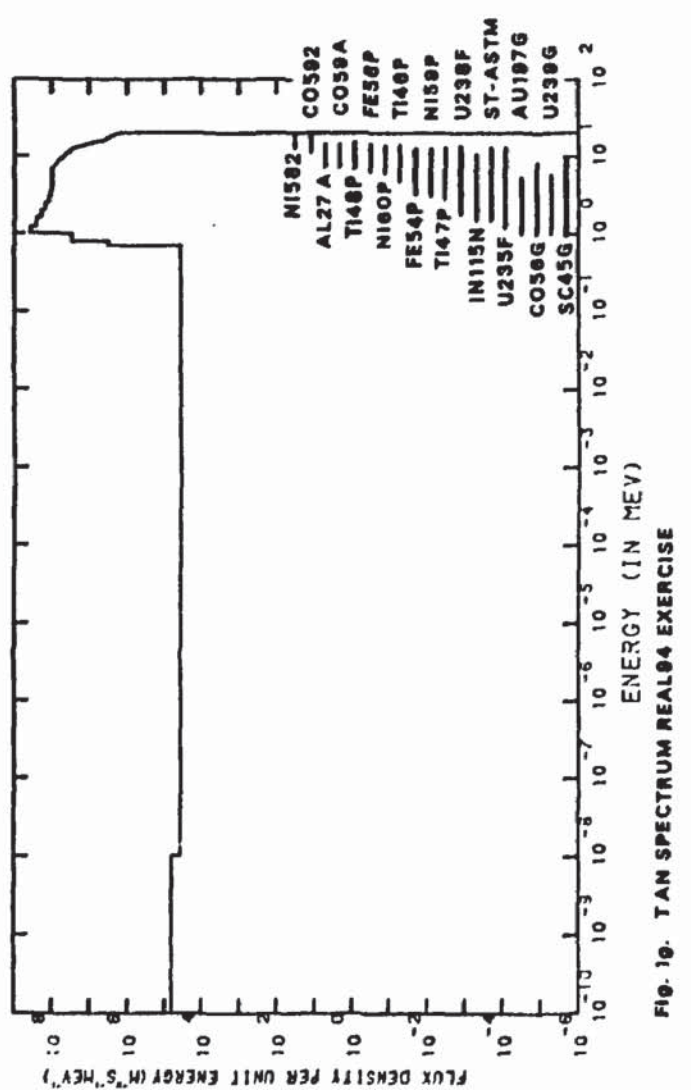


Fig. 19. TAN SPECTRUM REAL84 EXERCISE

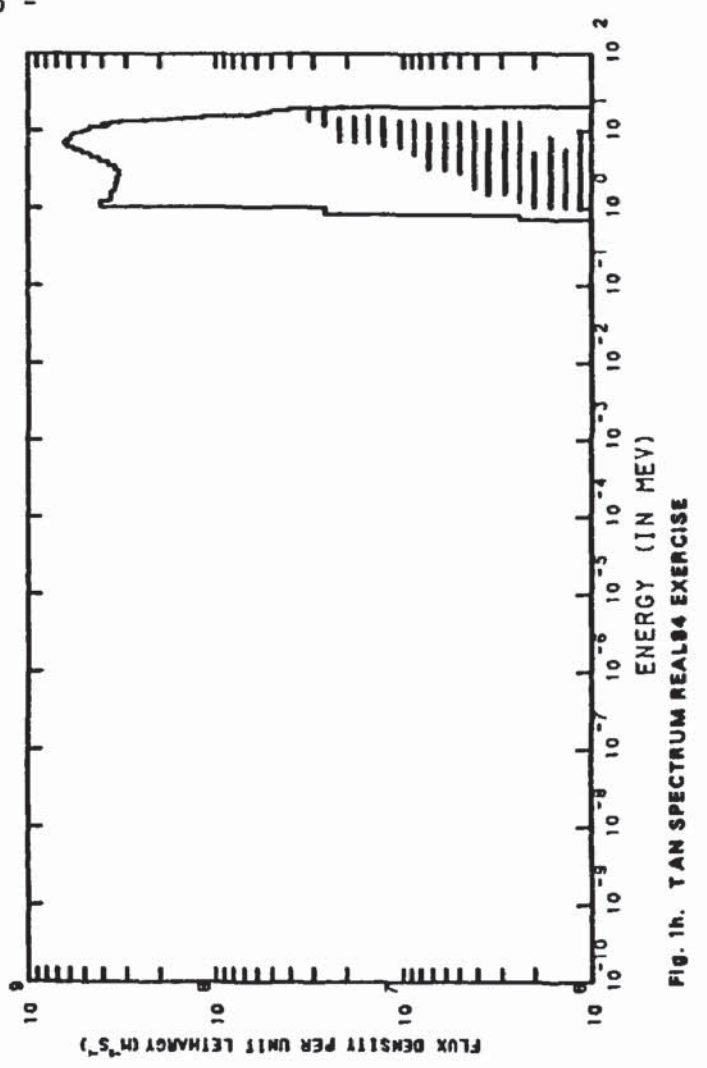


Fig. 1h. TAN SPECTRUM REAL84 EXERCISE

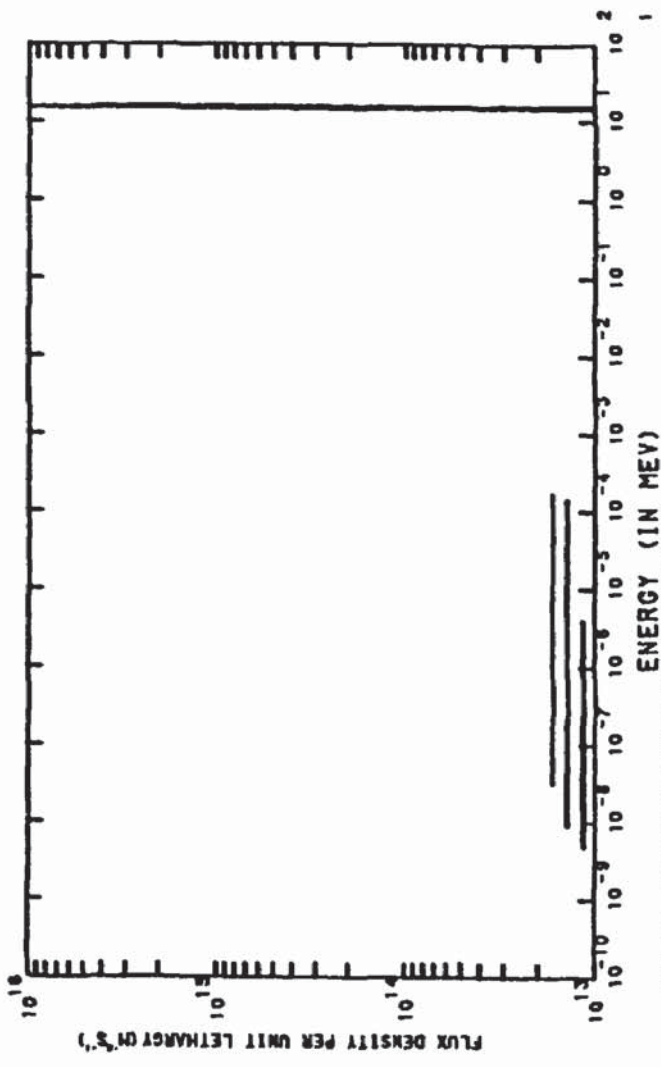


Fig. 1j. RTN SPECTRUM REAL84 EXERCISE

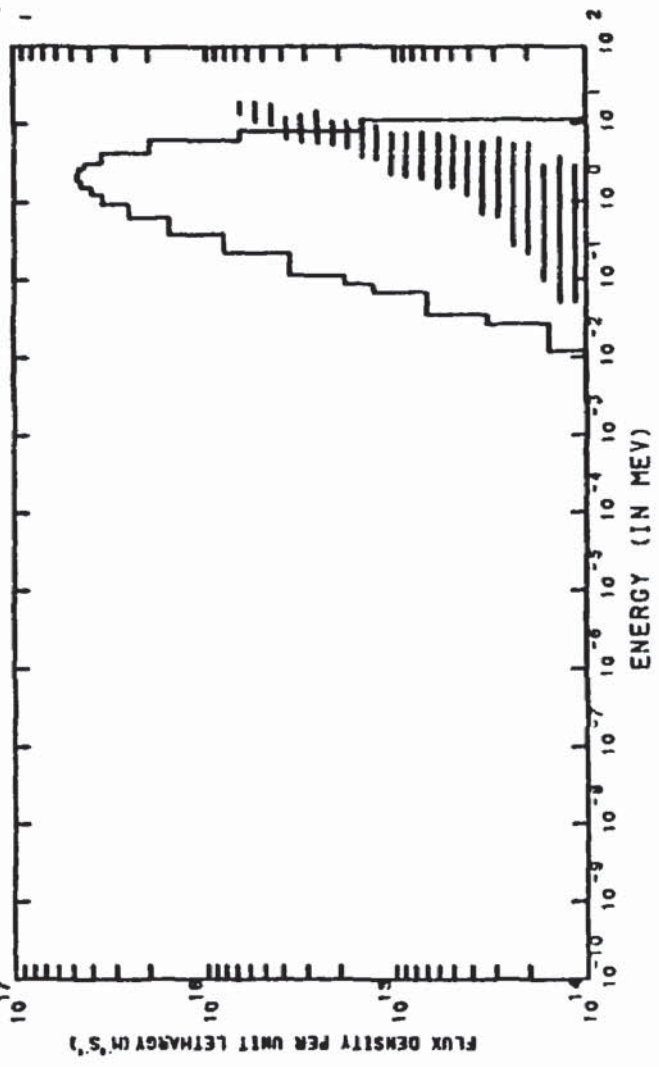


Fig. 1i. RTN SPECTRUM REAL84 EXERCISE

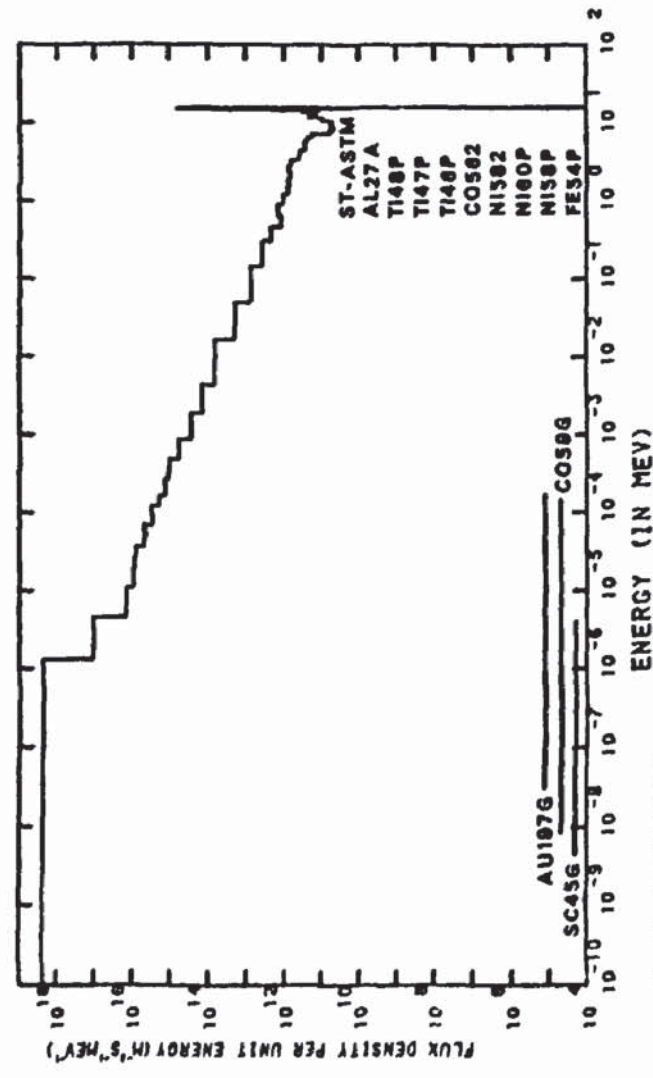


Fig. 1k. U35 SPECTRUM REAL84 EXERCISE

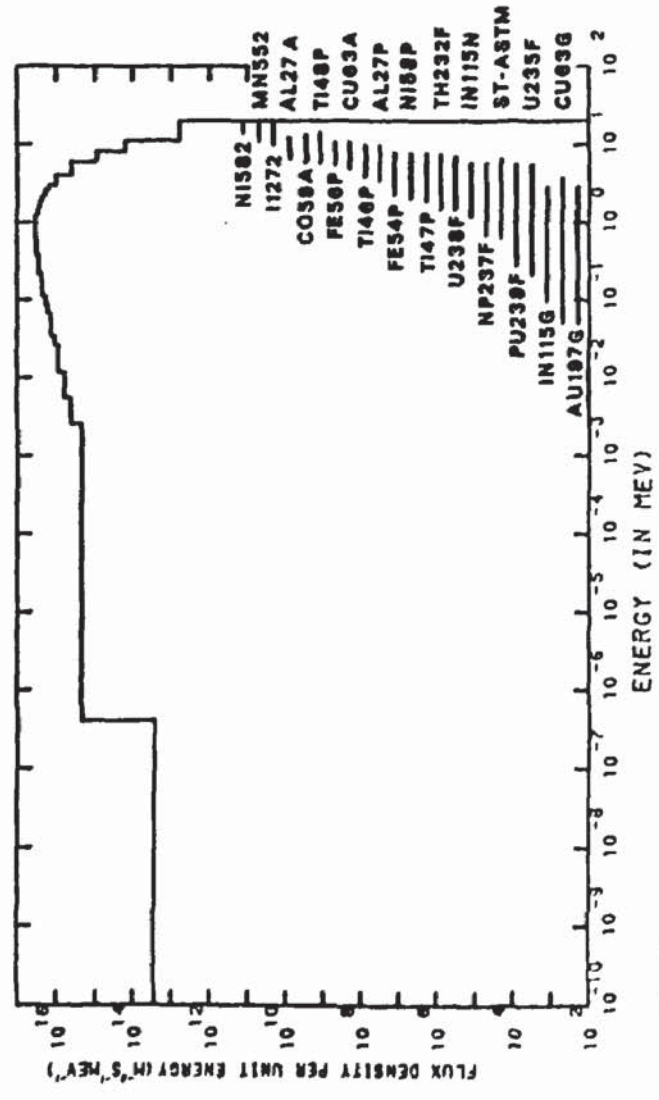


Fig. 1l. U35 SPECTRUM REAL84 EXERCISE

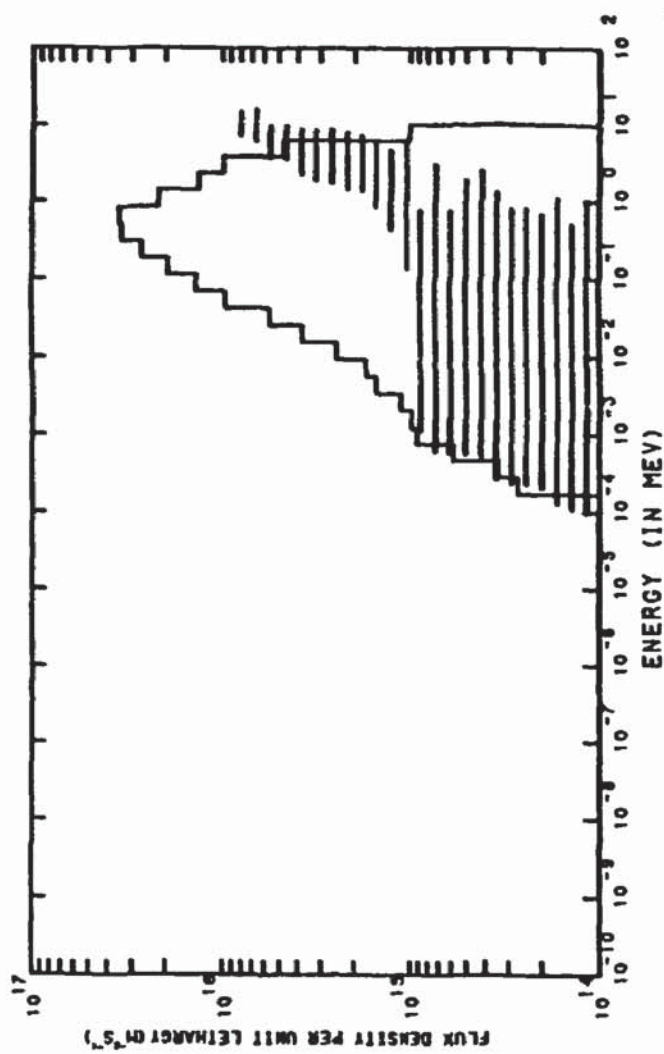


Fig. 1n. CFR SPECTRUM REAL84 EXERCISE

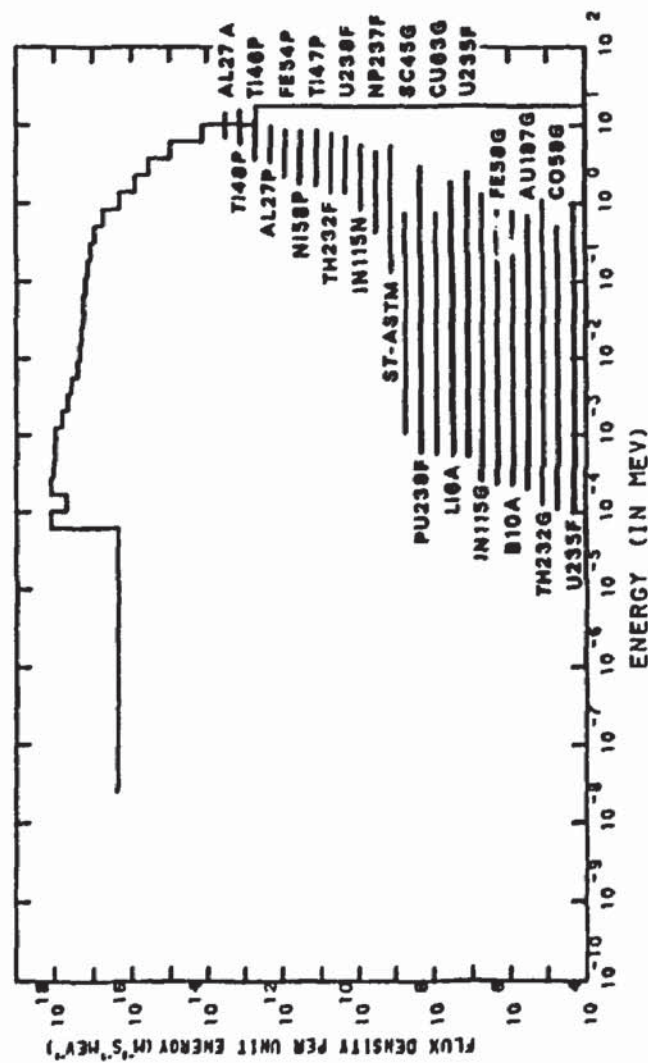


Fig. 1m. CFR SPECTRUM REAL84 EXERCISE

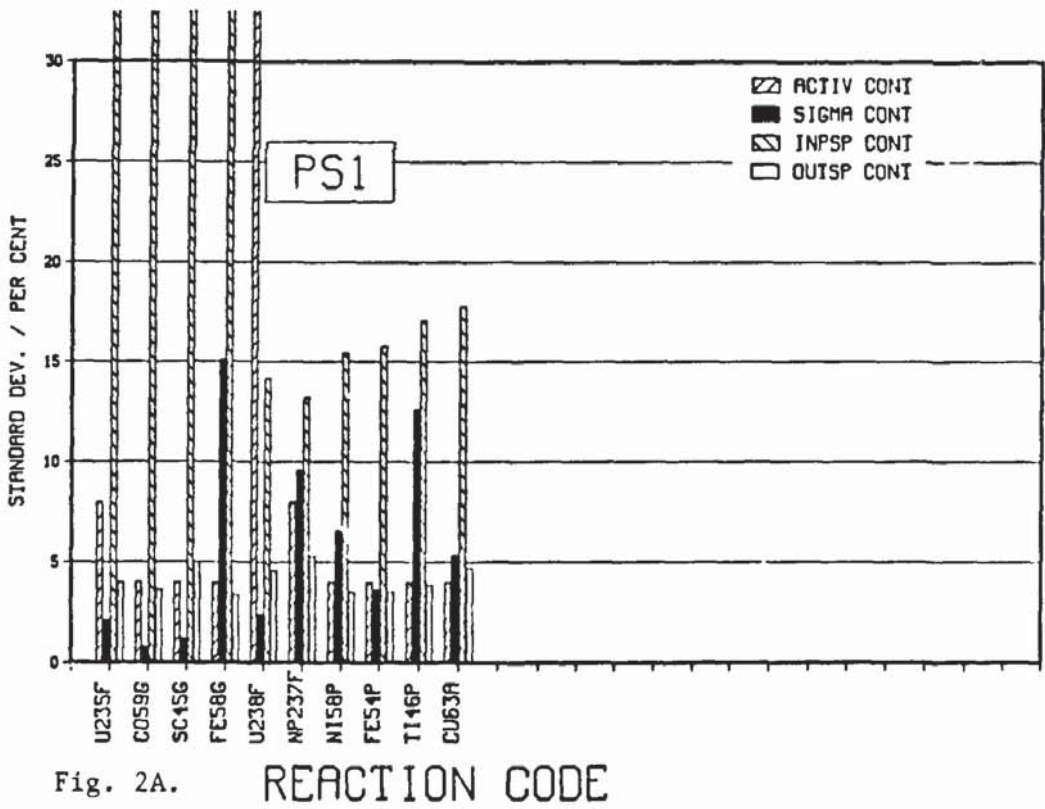
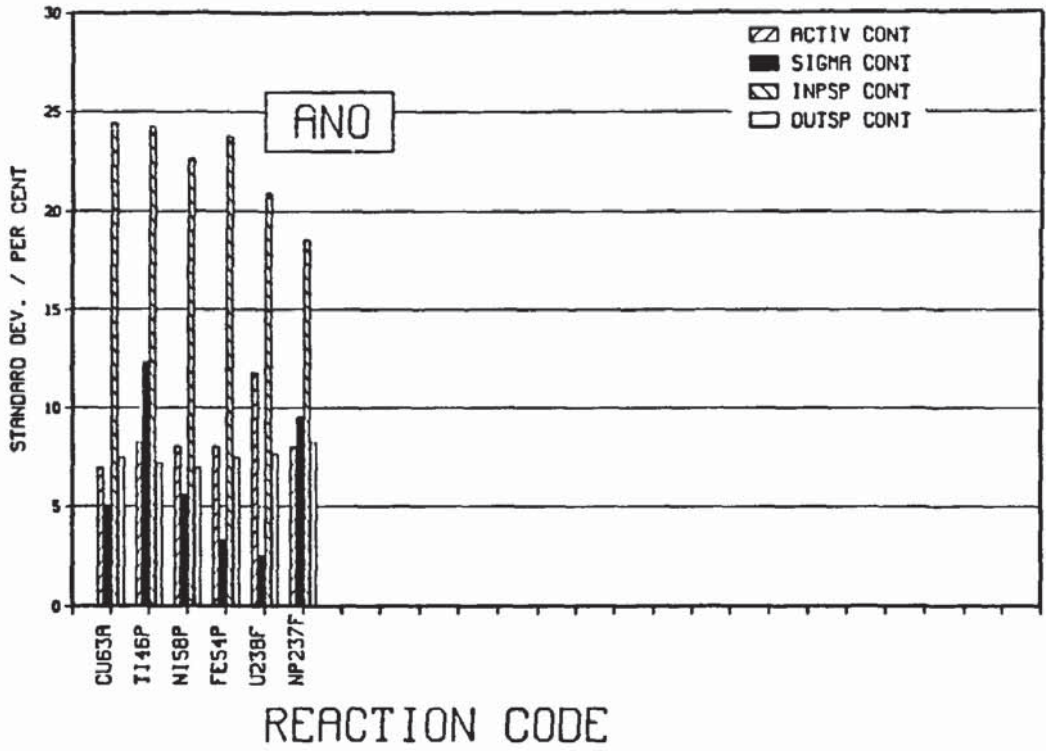


Fig. 2A.

REACTION CODE

Fig. 2. Importance of contributions to the reaction rate uncertainties.

For each reaction rate the uncertainty contributions of measured activity, the reaction cross-section, the input spectrum, and the output spectrum are shown.

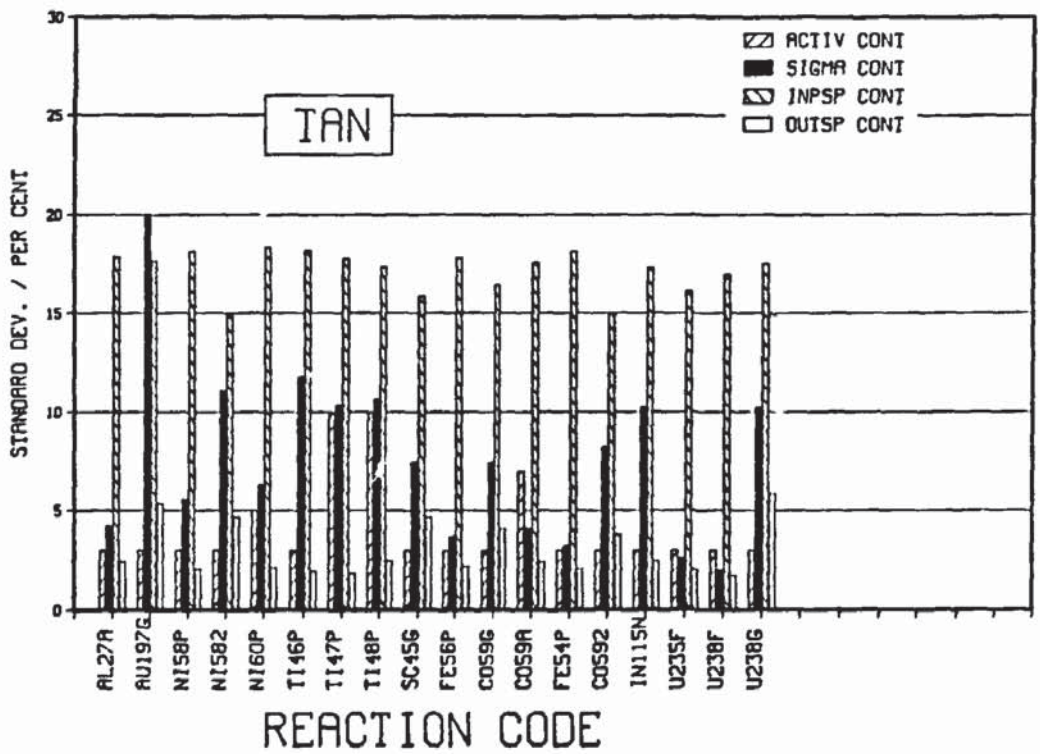
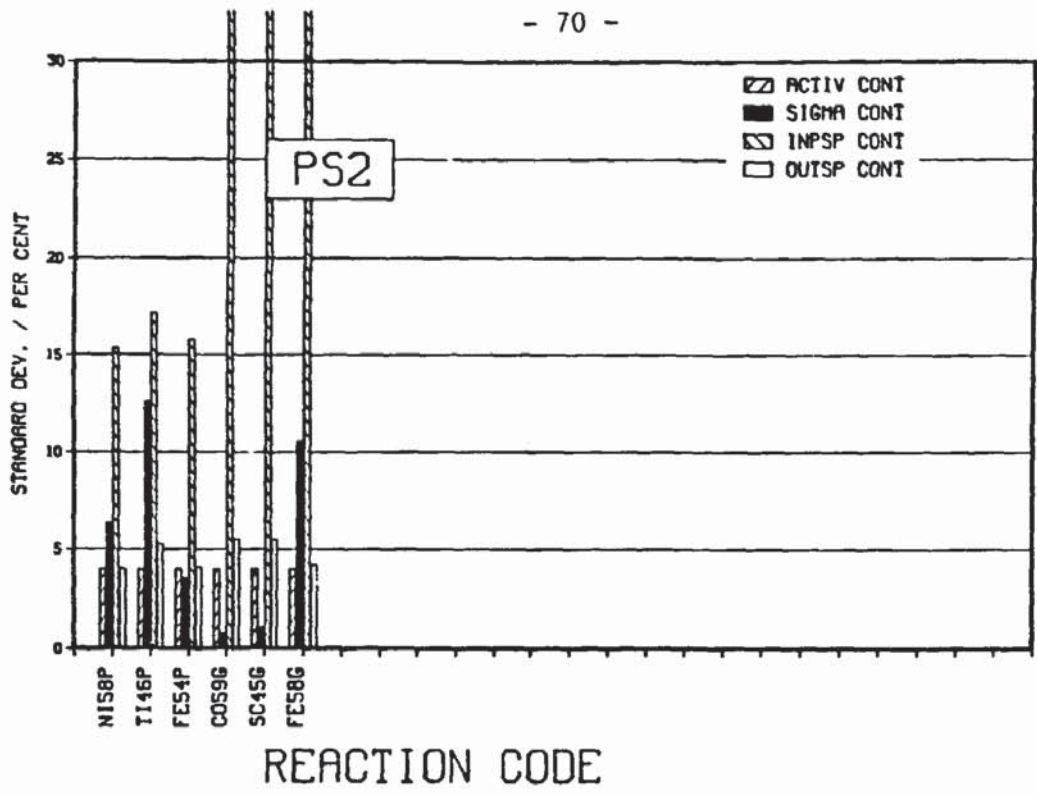


Fig. 2B.

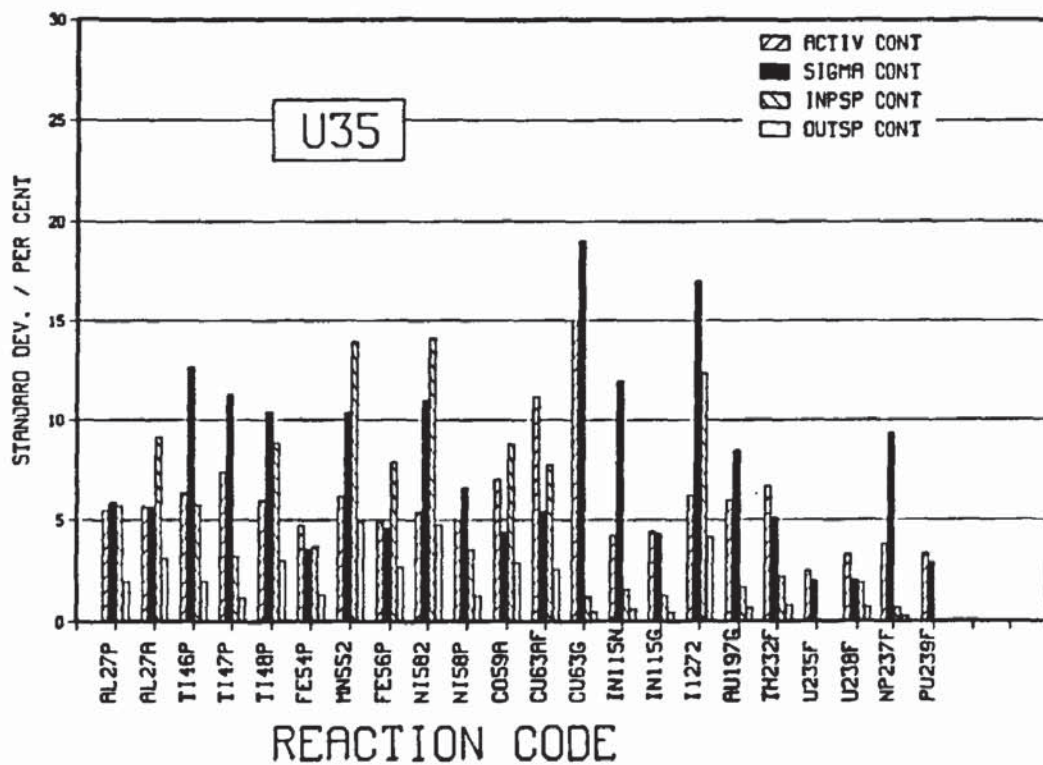
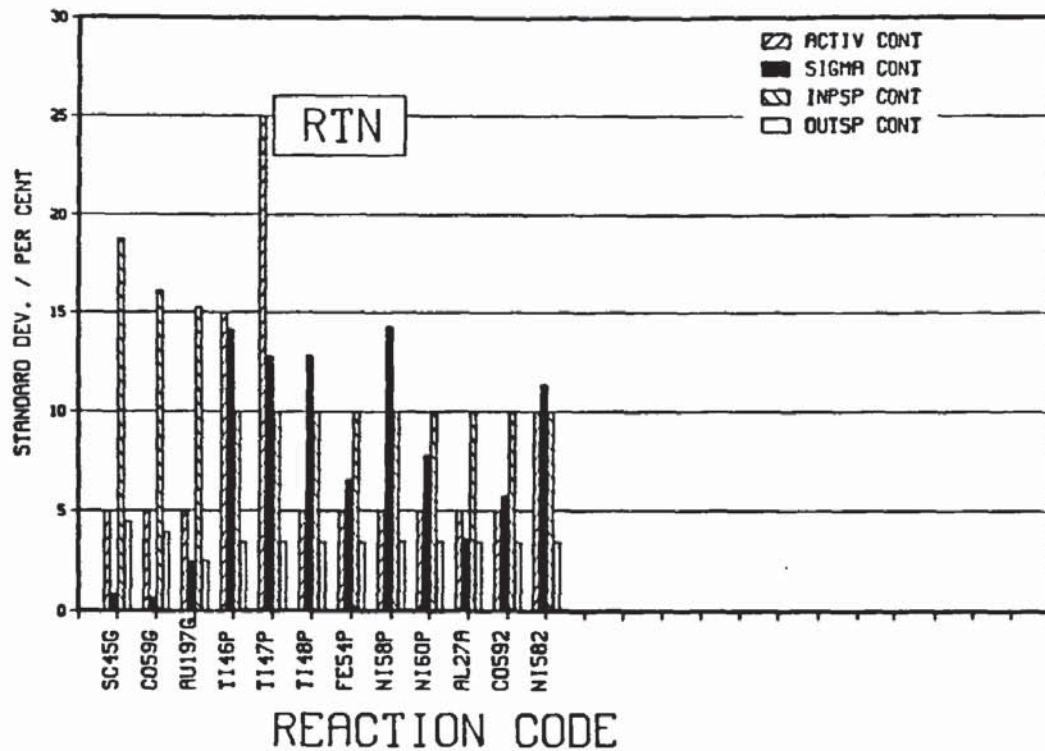


Fig. 2C.

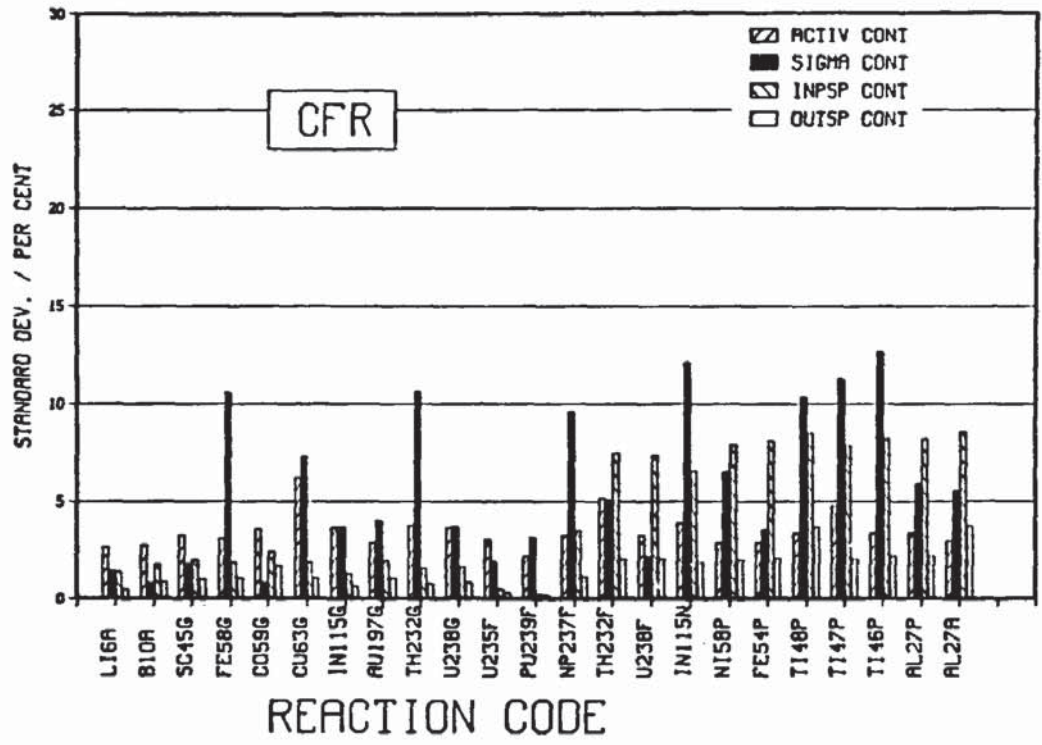


Fig. 2D.

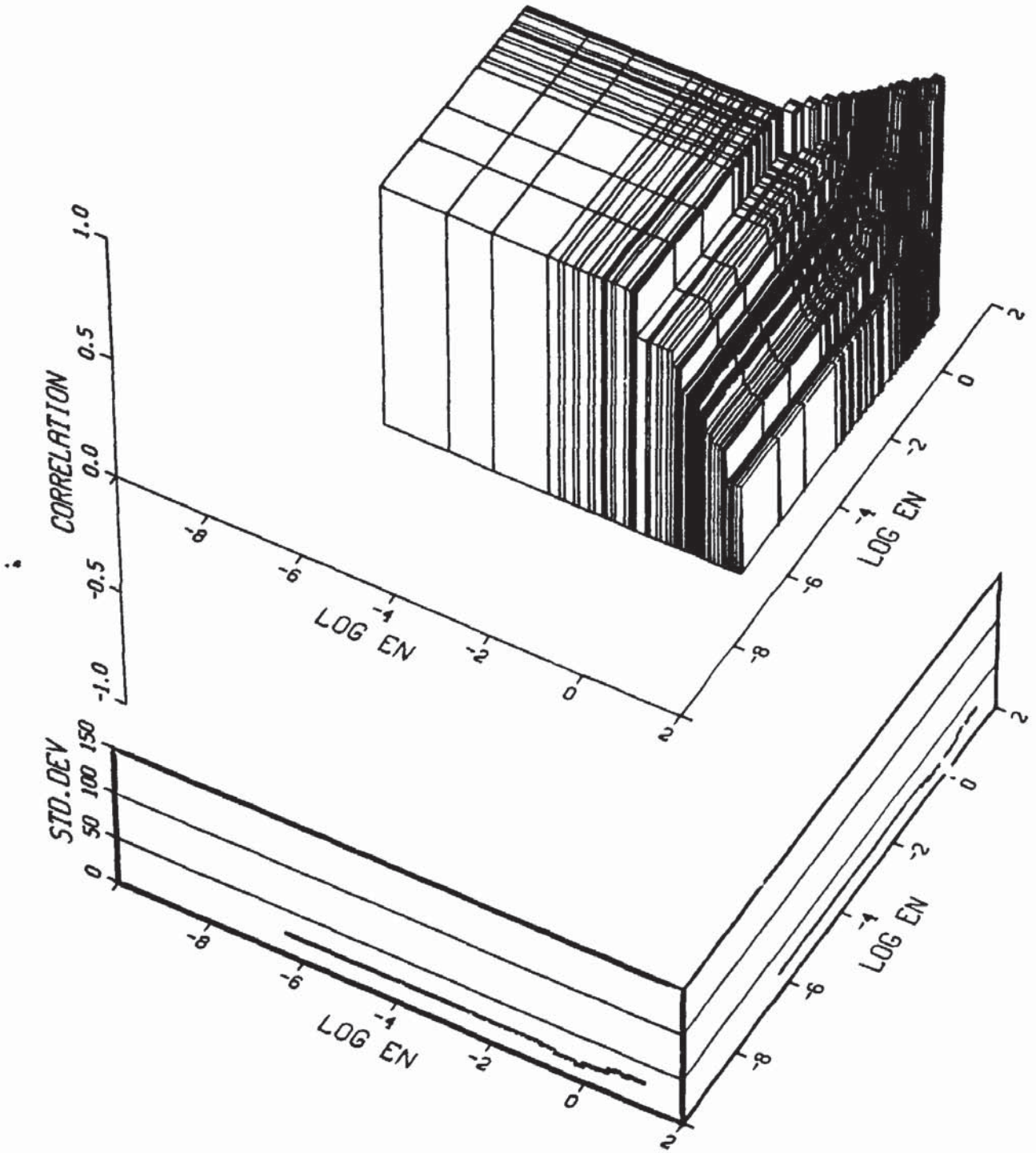


Fig. 3. Input neutron spectrum covariance data for ANO.

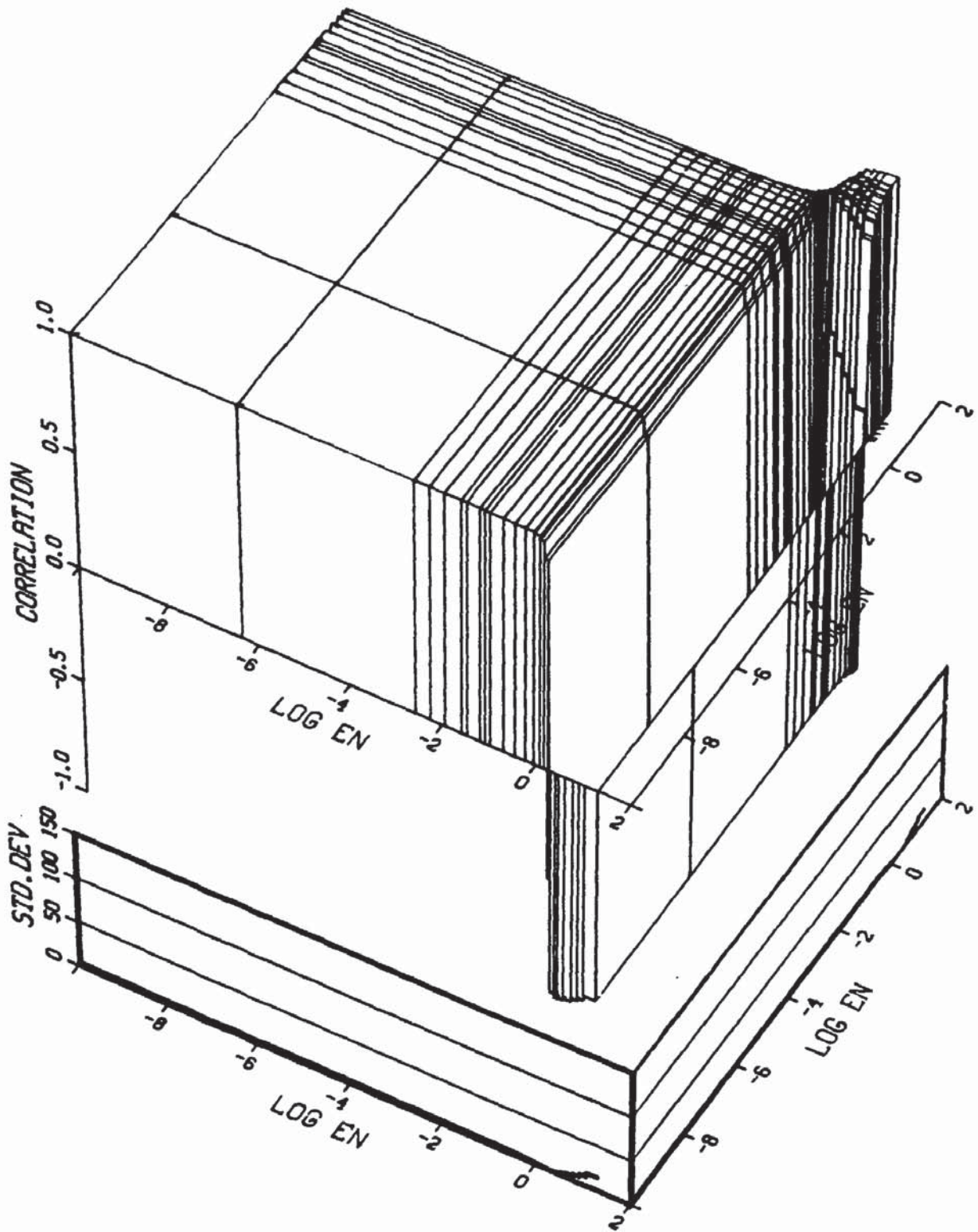


Fig. 4. Input neutron spectrum covariance data for U35.

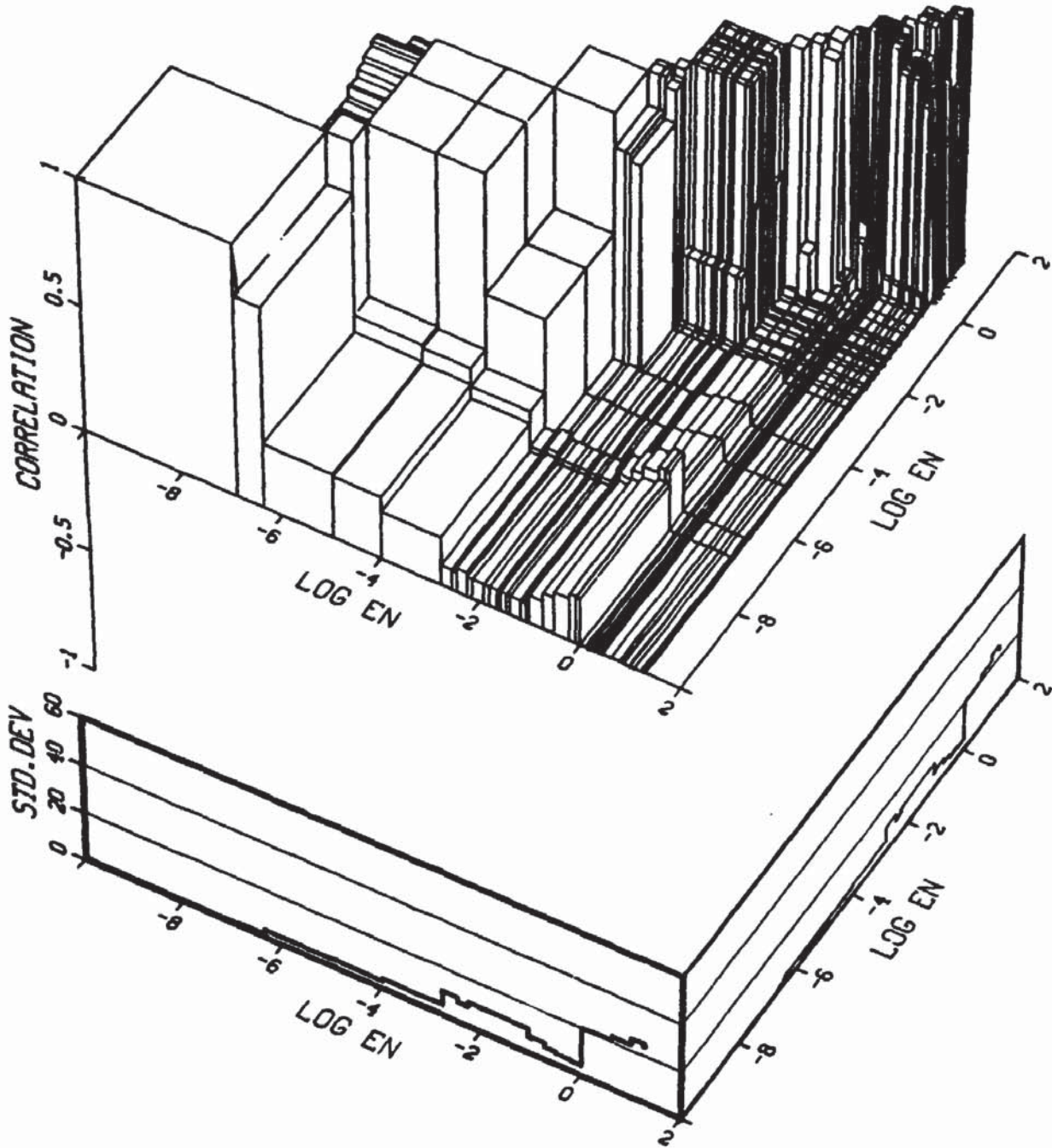


Fig. 5. CROSS SECTION COVARIANCE DATA FOR AU197G

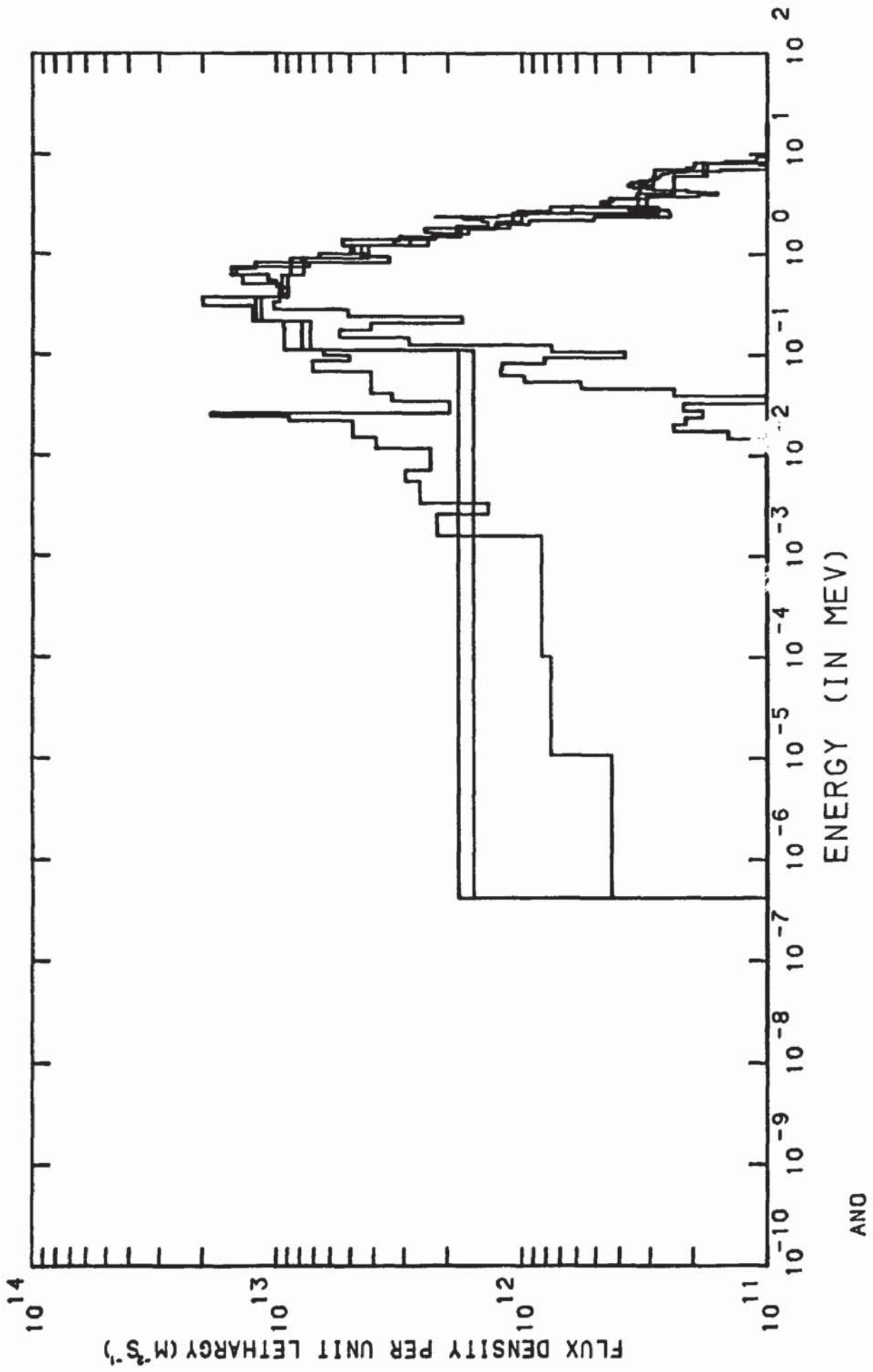
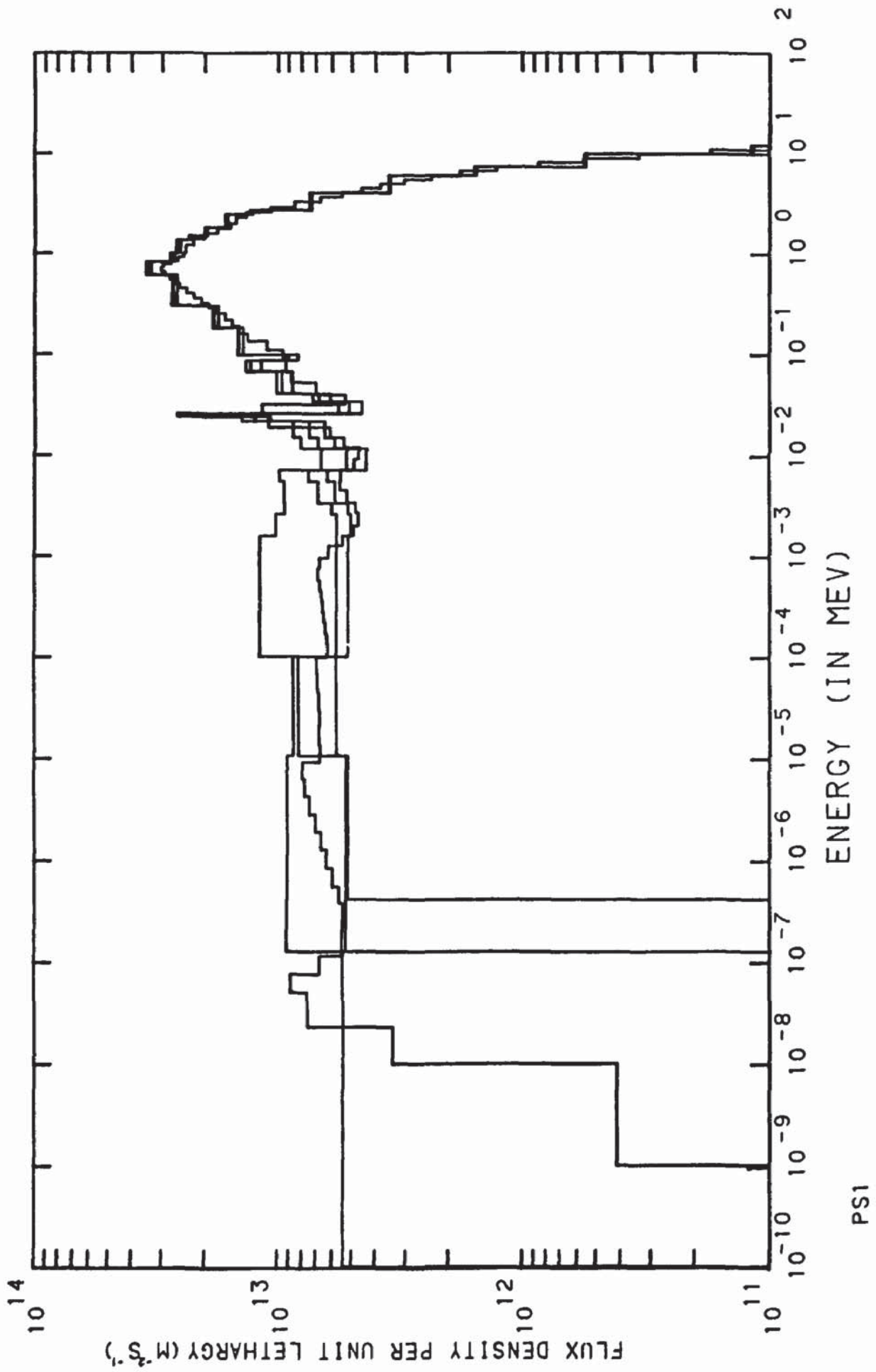


Fig. 6a. All output spectra for ANO.



PSI
Fig. 6b All output spectra for PSI.

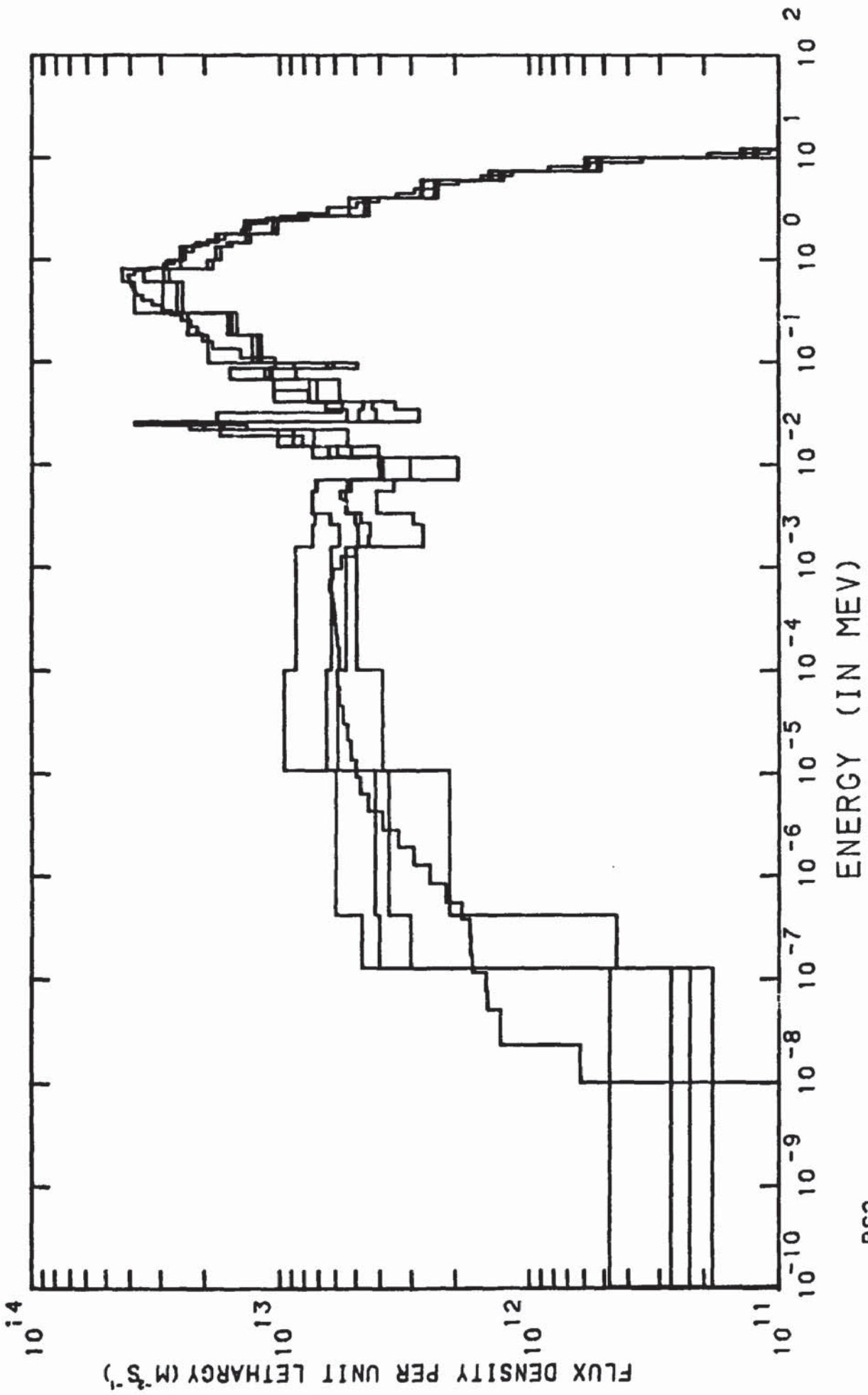


Fig. 6c. All output spectra for PS2.

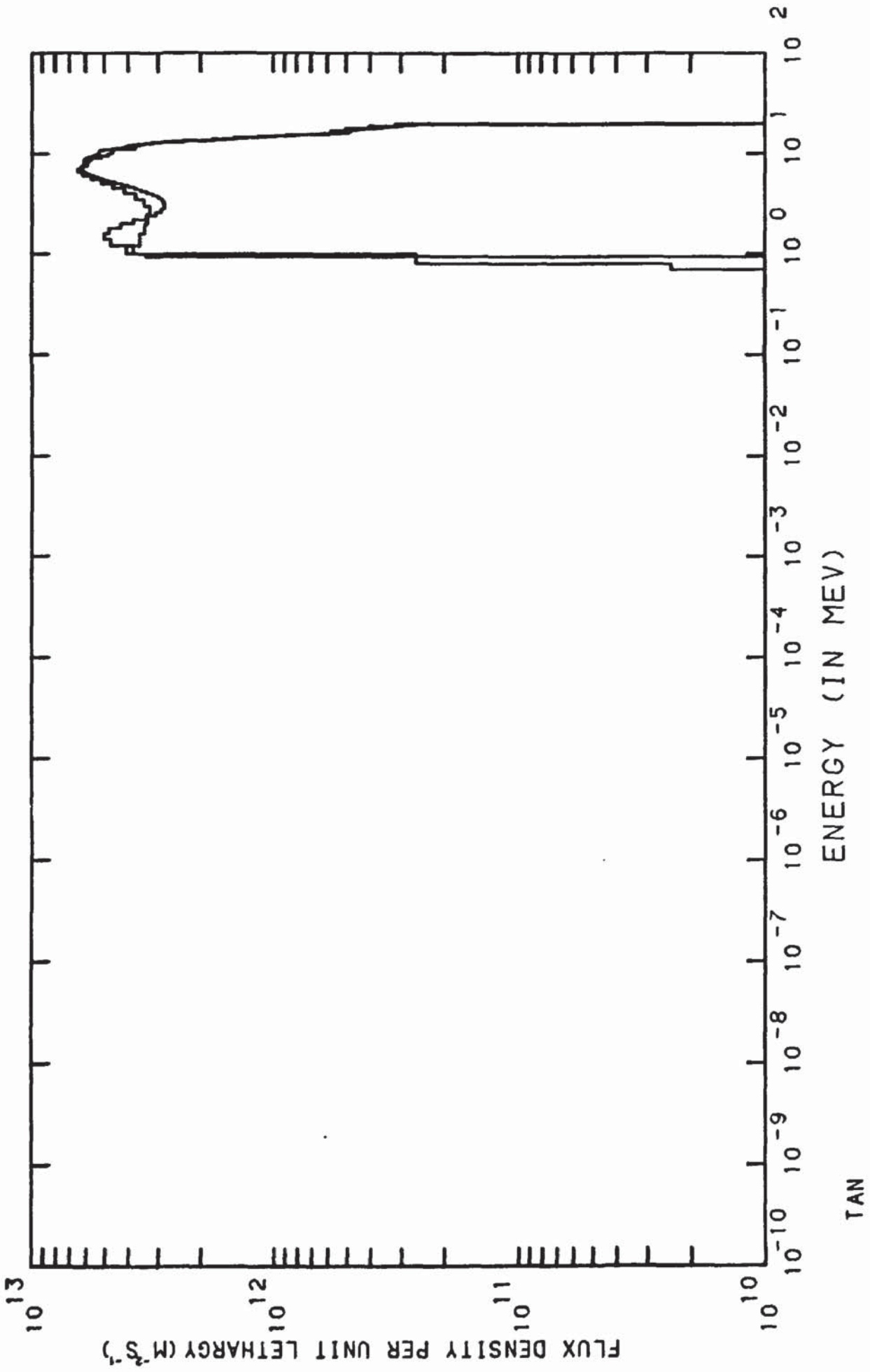


Fig. 6d. All output spectra for TAN.

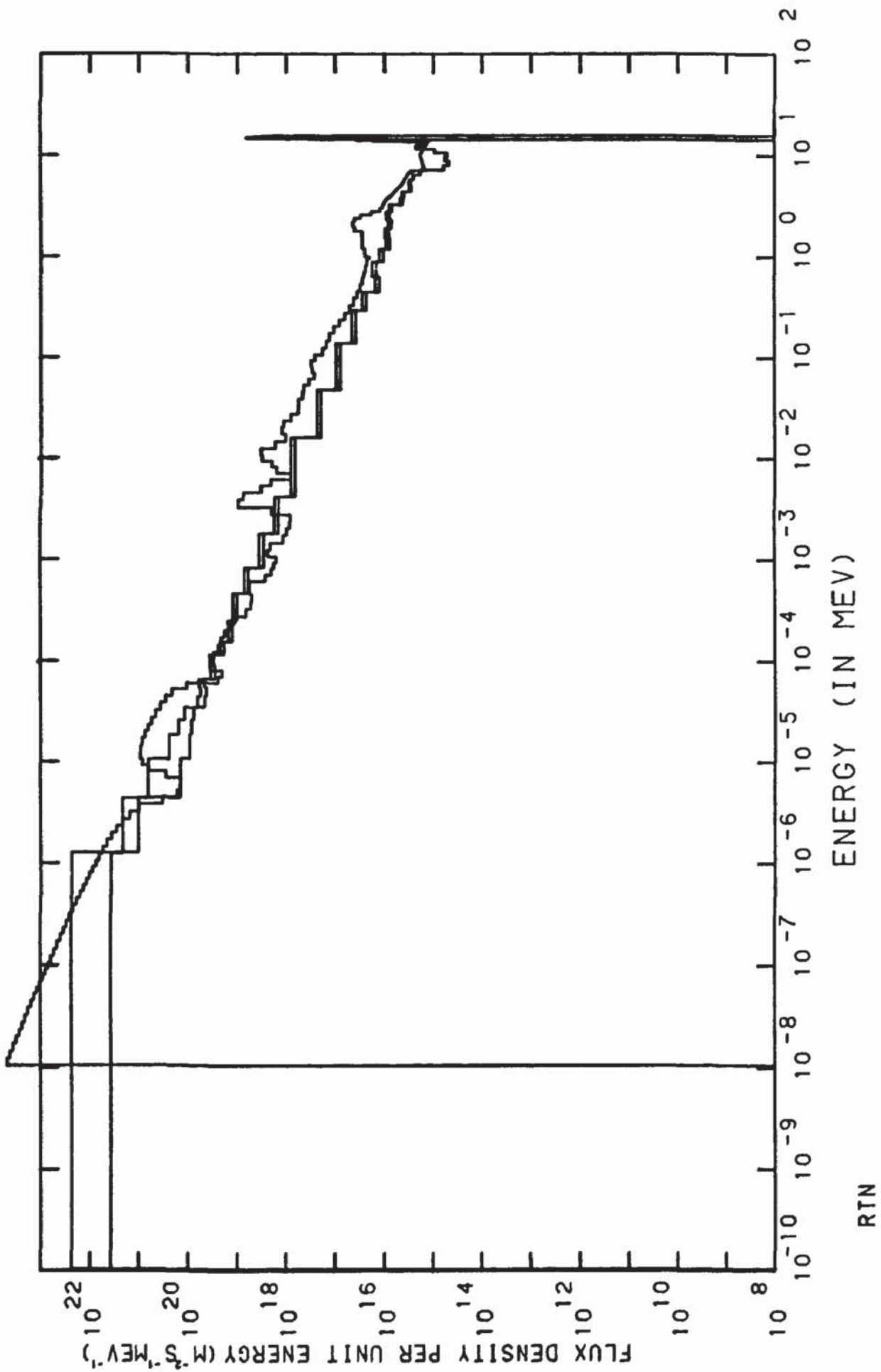
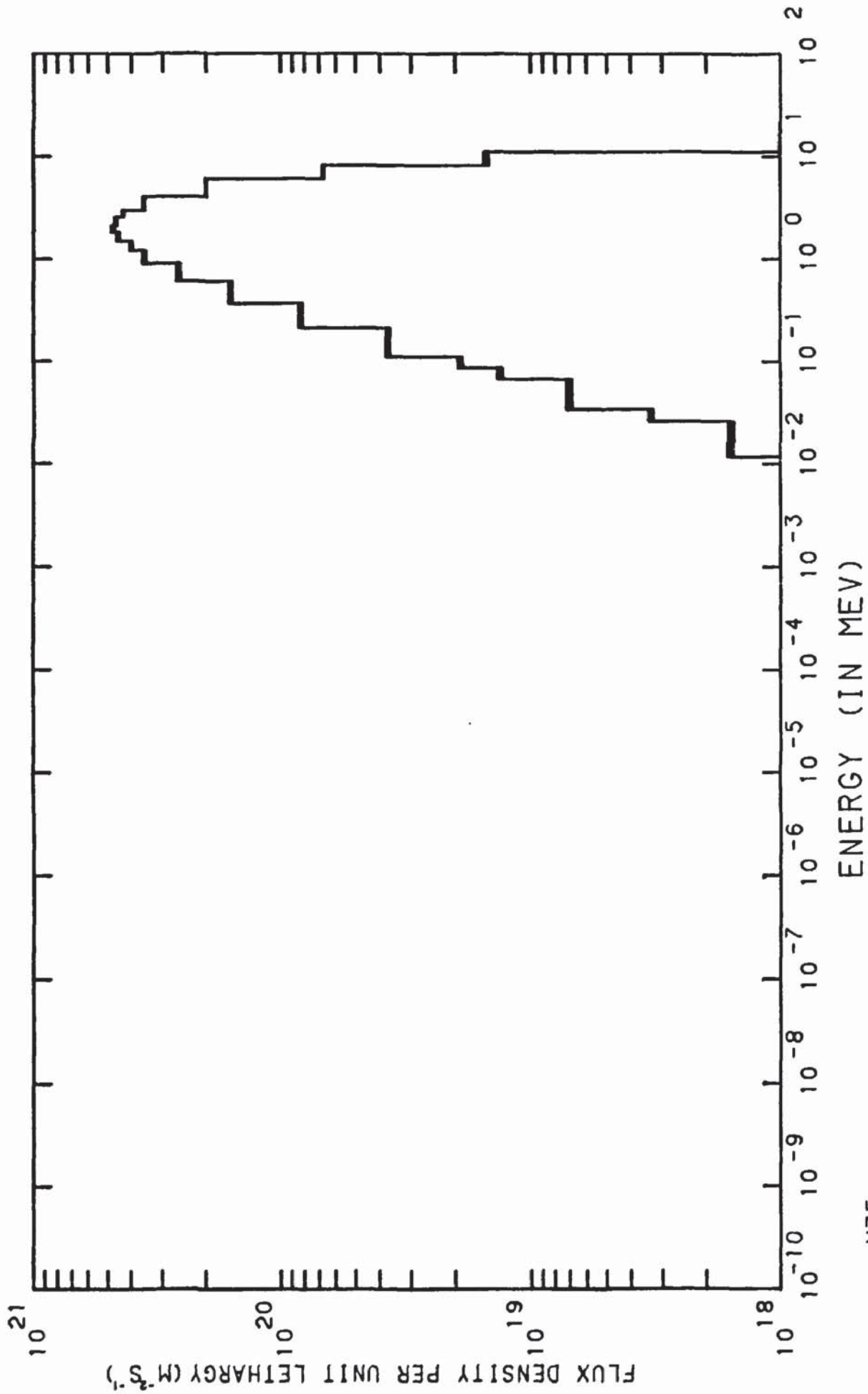


Fig. 6e. All output spectra for RTN.



U35

Fig. 6f. All output spectra for U35.

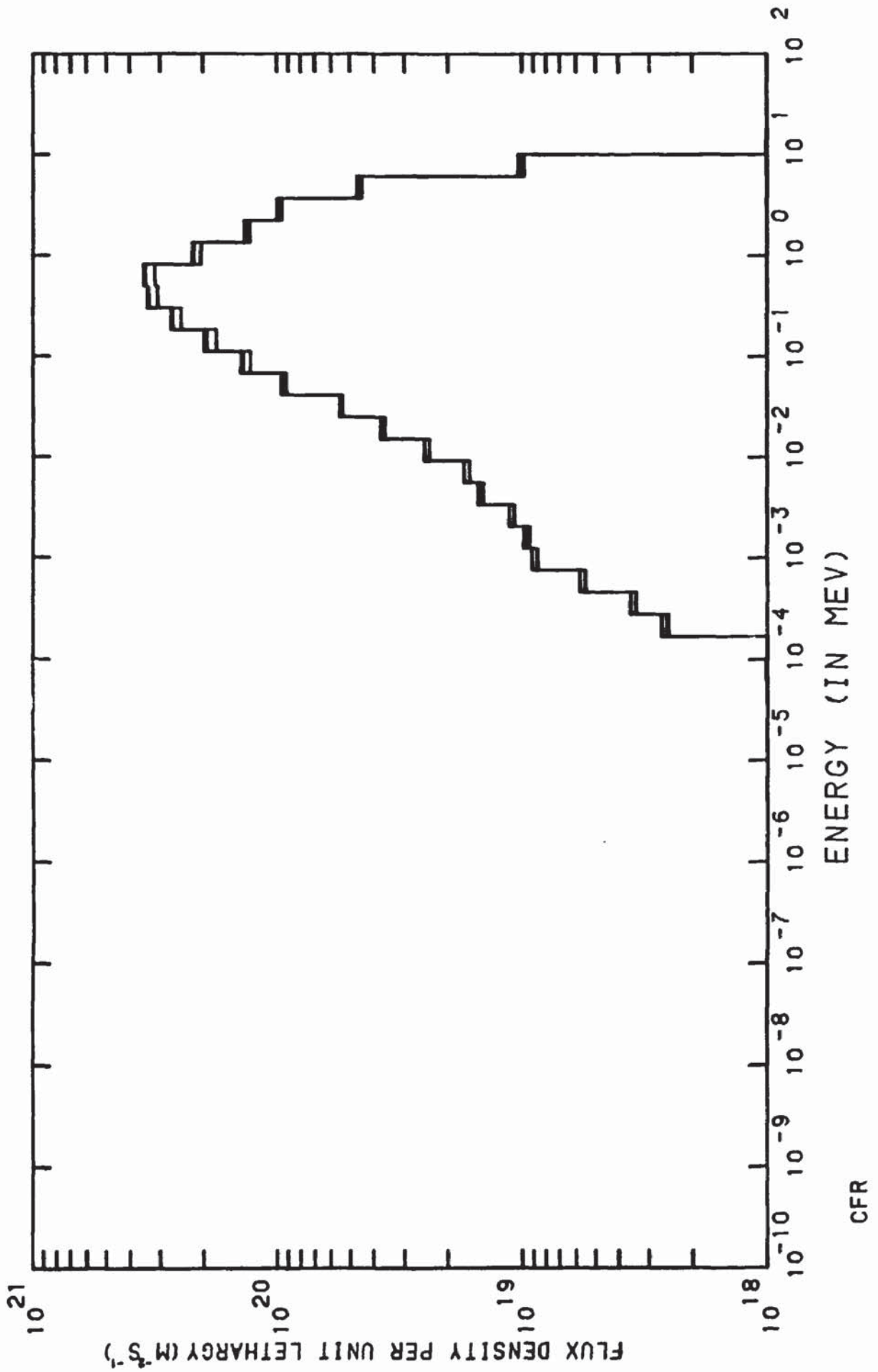


Fig. 6g. All output spectra for CFR.

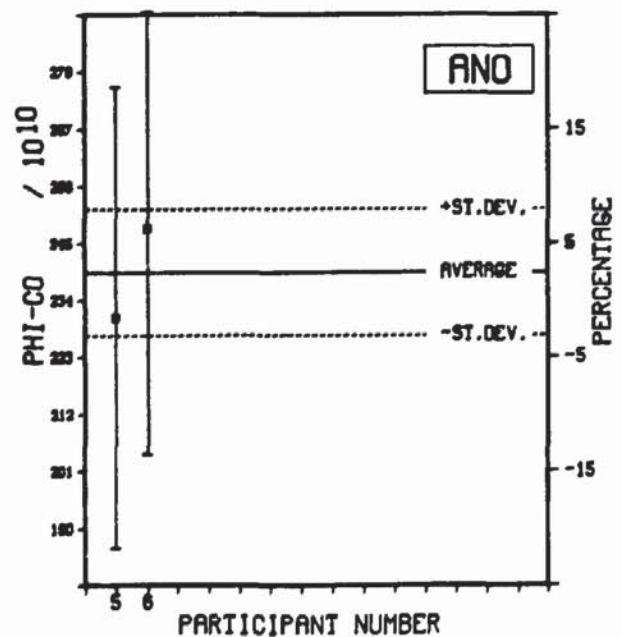
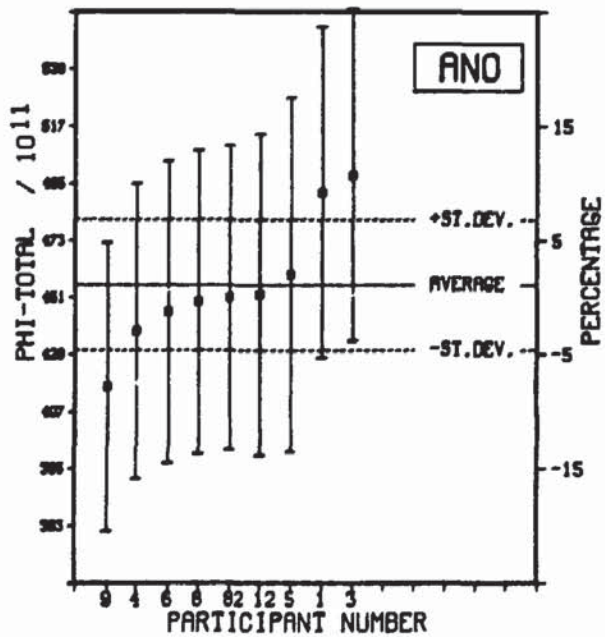
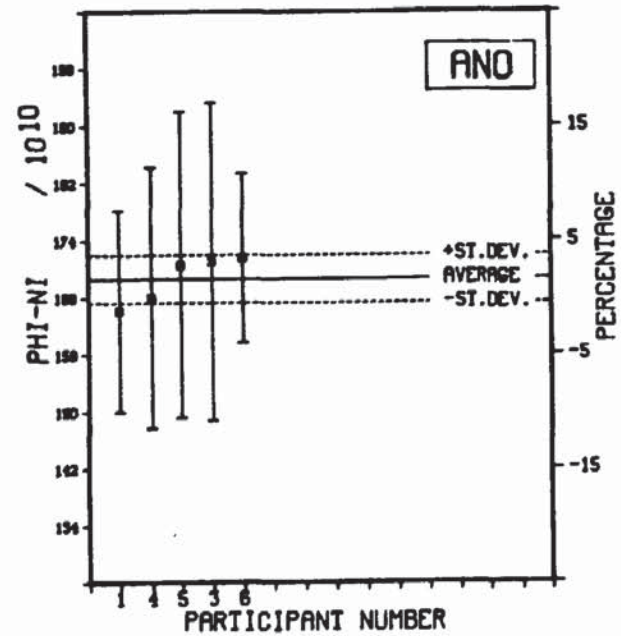
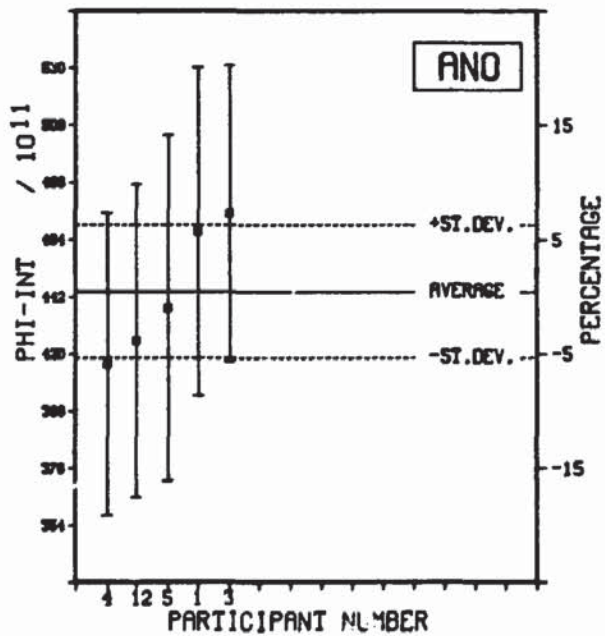
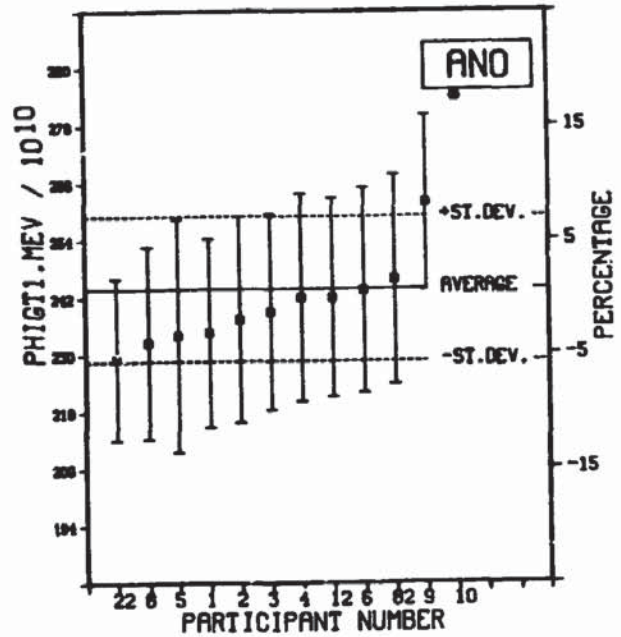
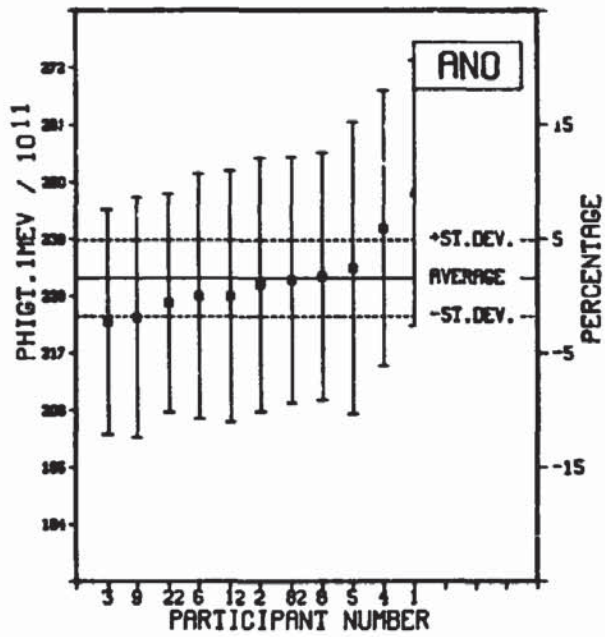


Fig. 7.a.1. ANO.

Fig. 7. Comparison of integral (damage) parameters calculated by the participants.

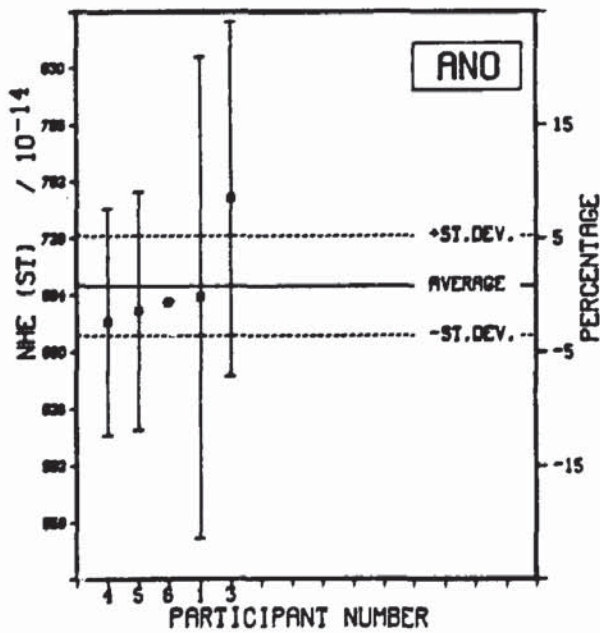
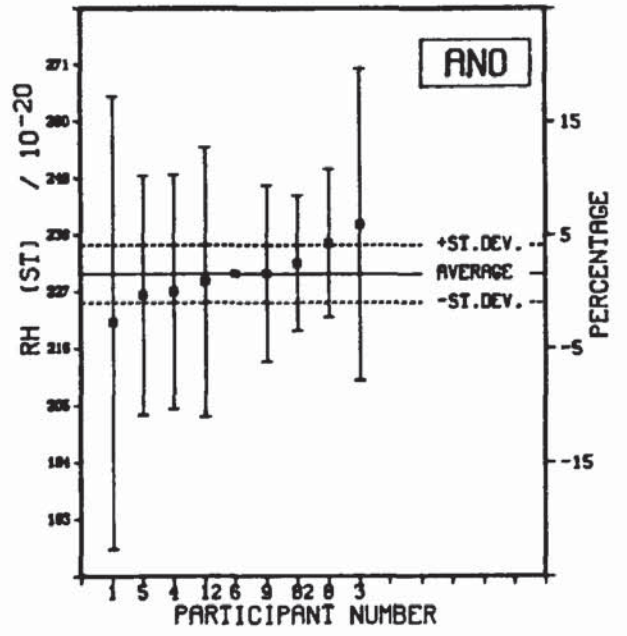
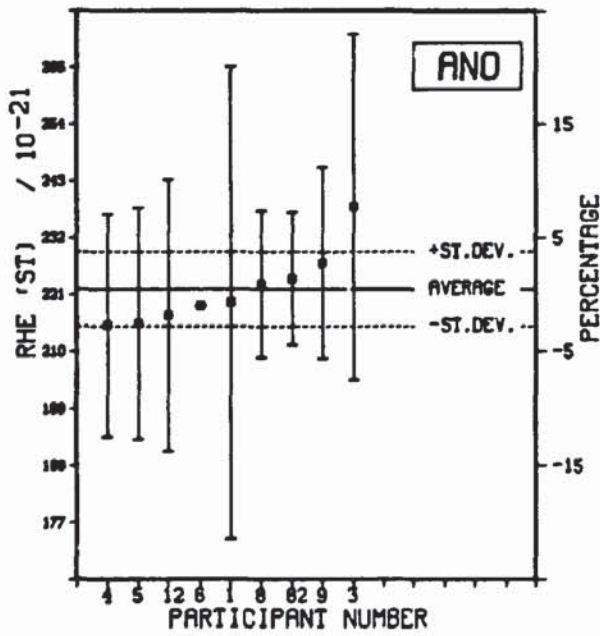
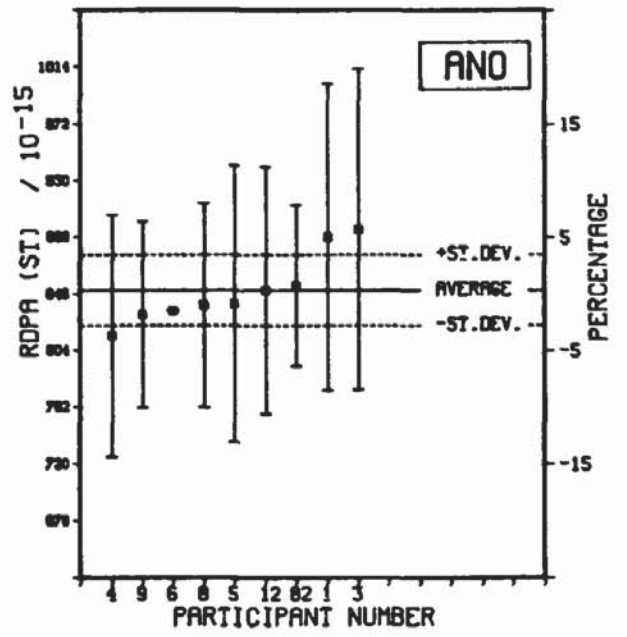
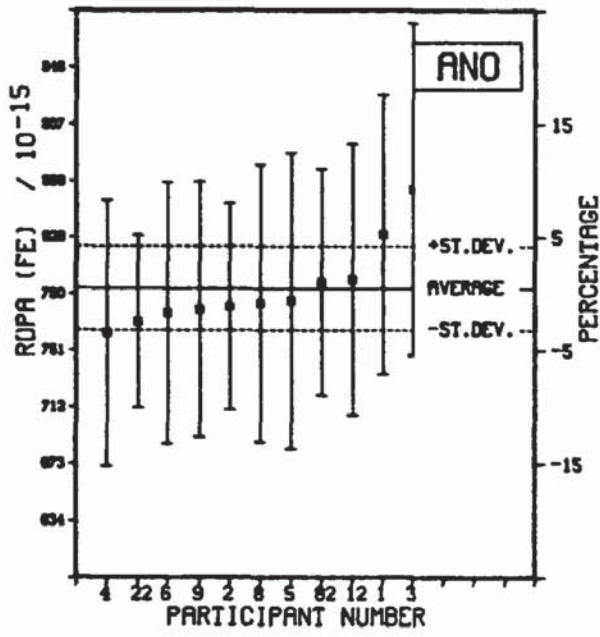


Fig. 7.a.2. ANO.

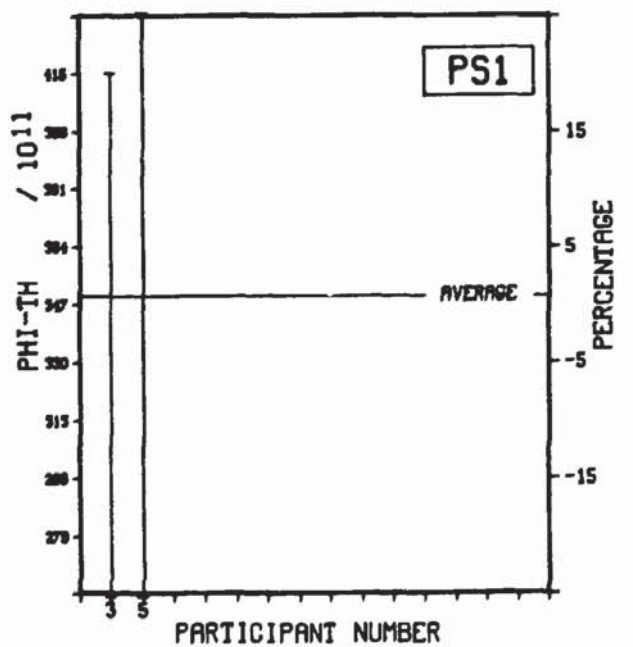
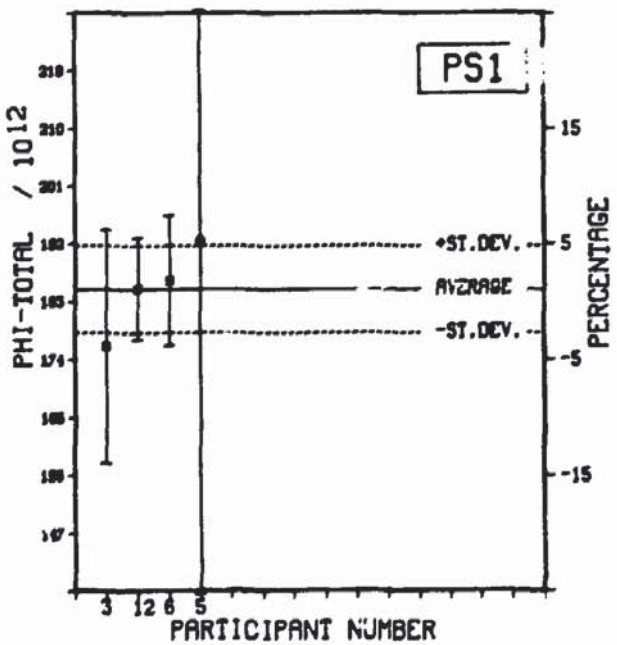
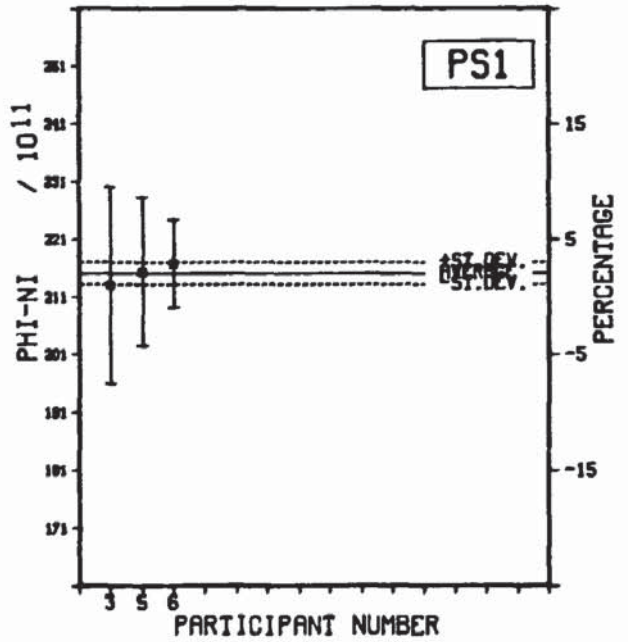
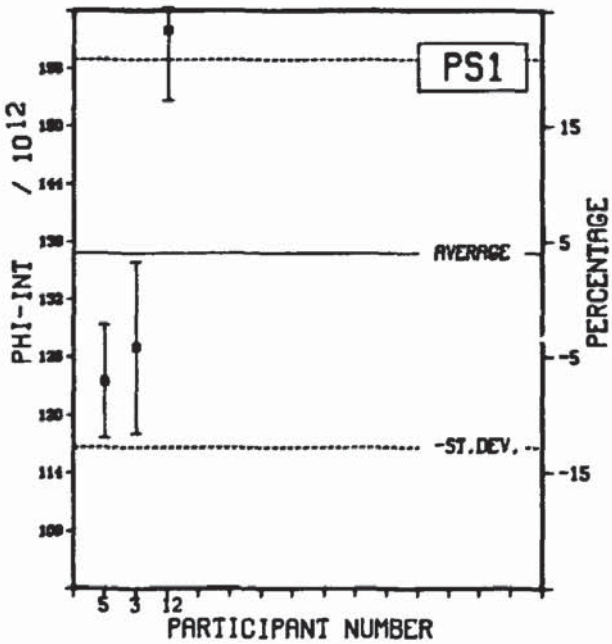
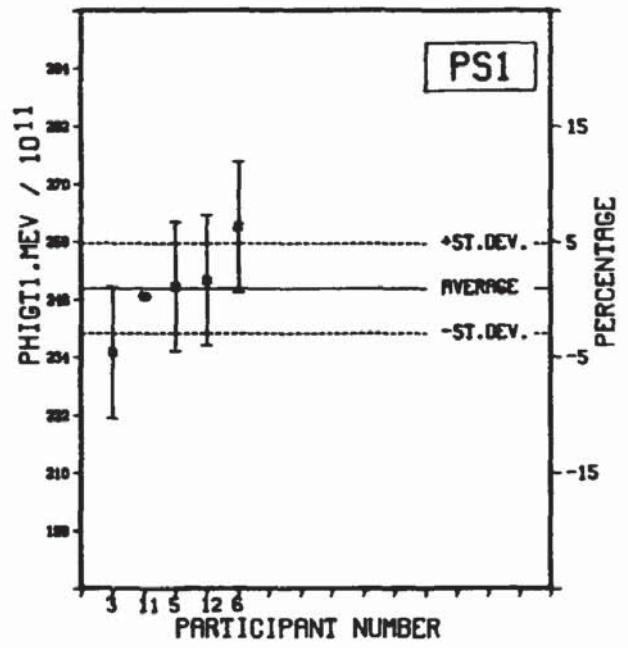
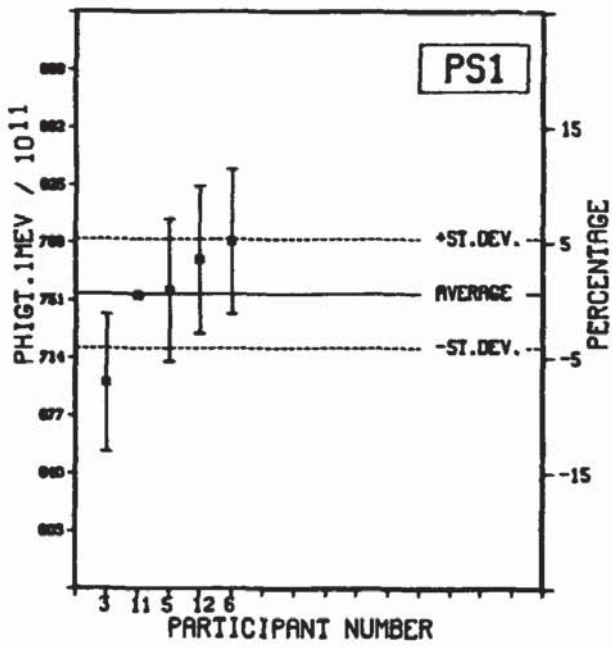


Fig. 7.bL PS1.

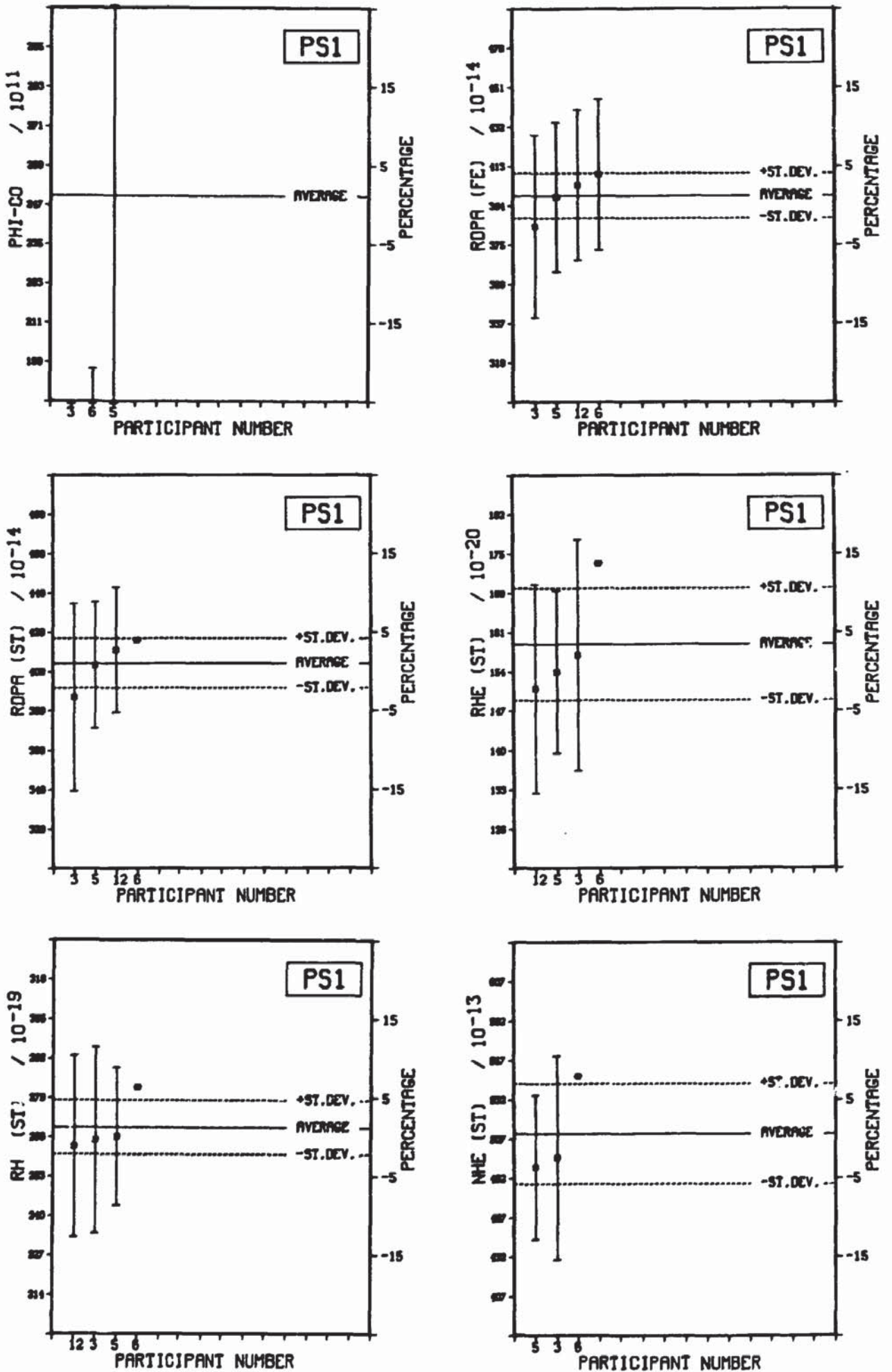


Fig. 7.b.2. PS1.

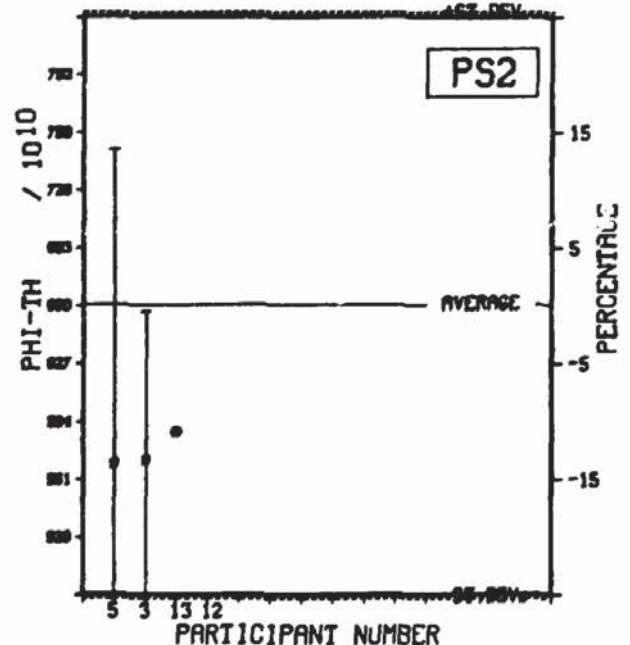
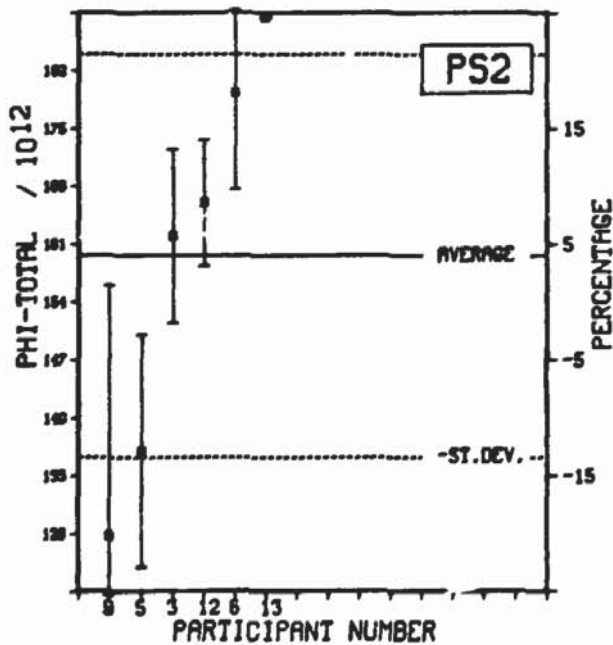
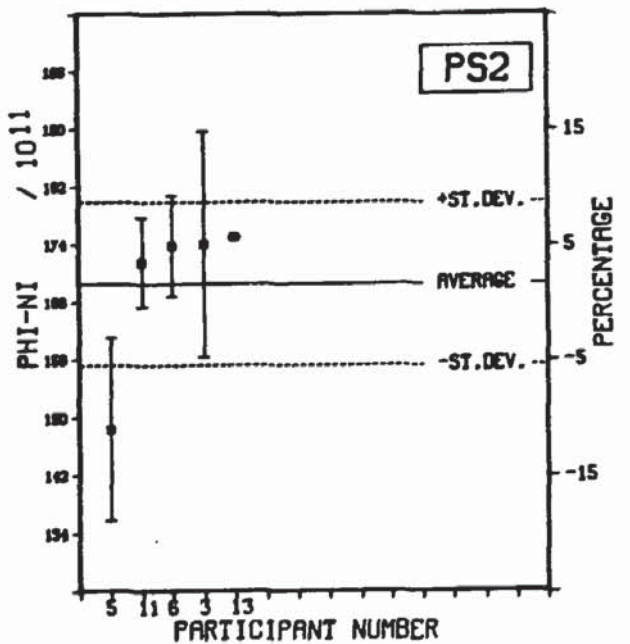
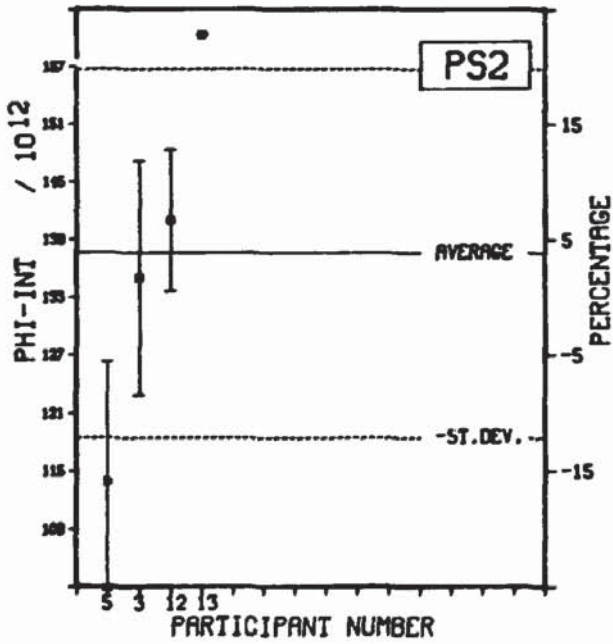
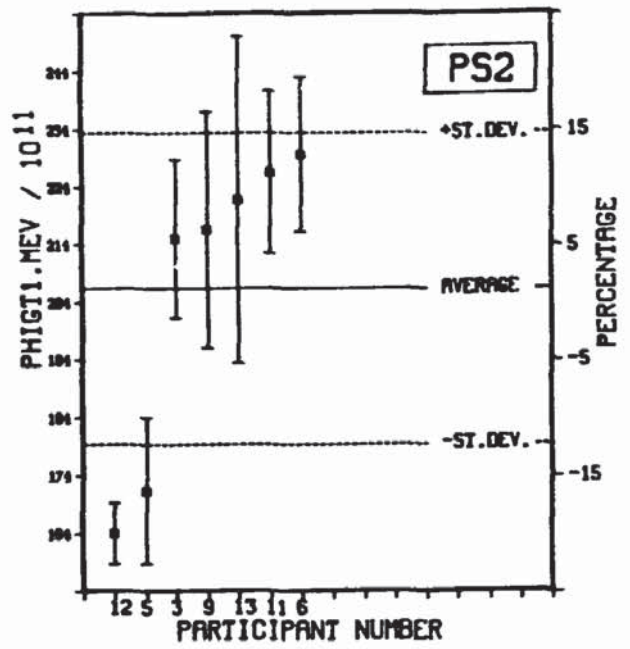
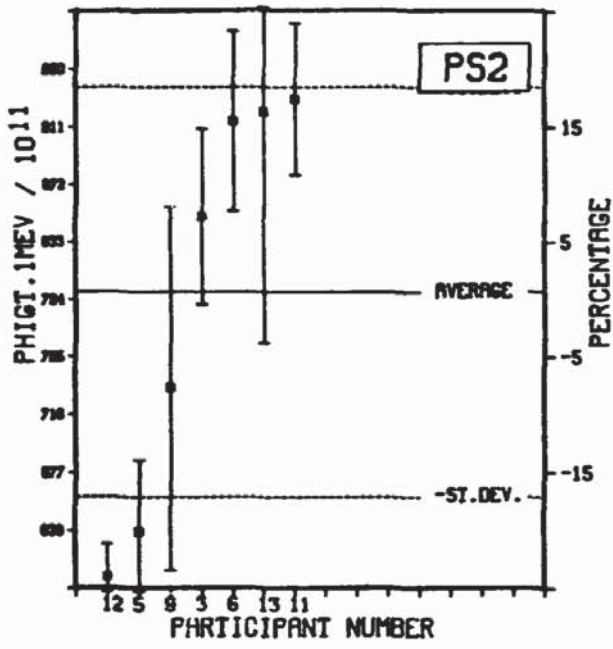


Fig. 7.c.1. PS2.

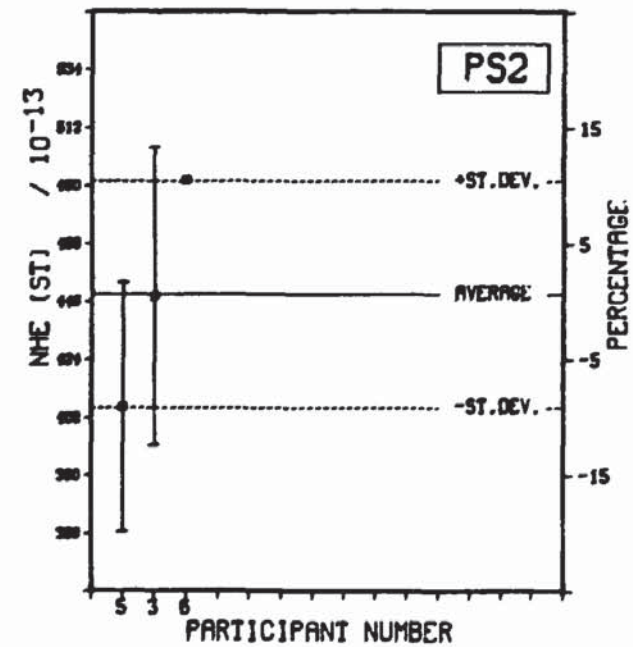
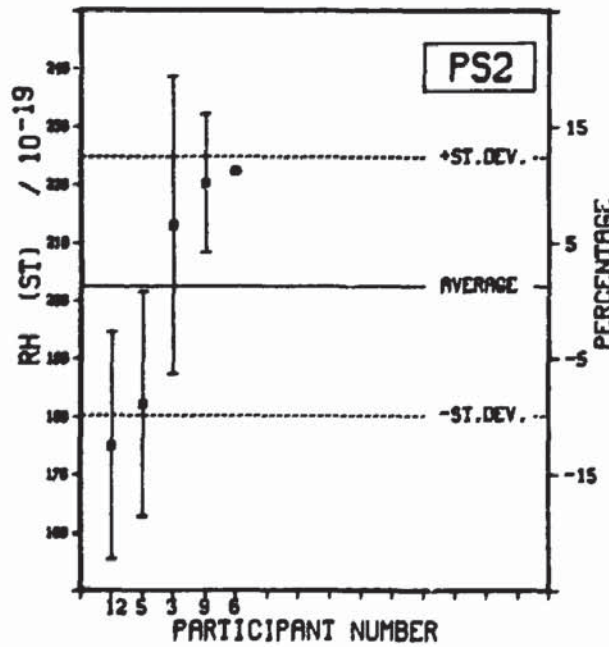
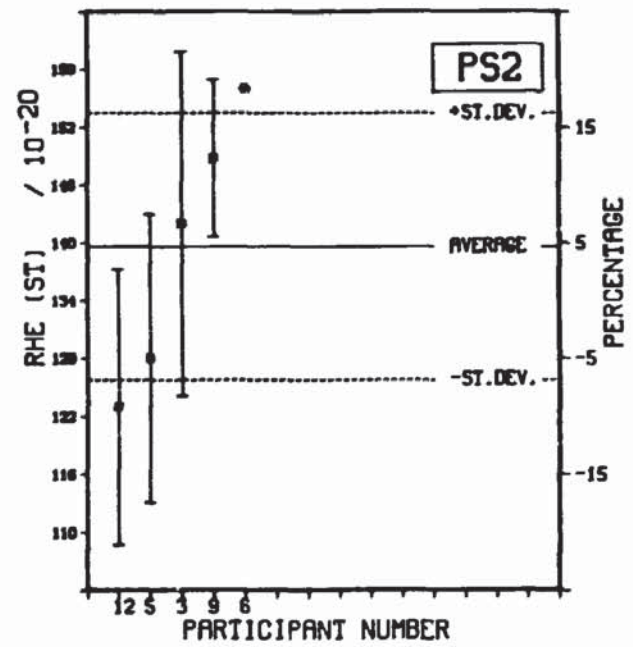
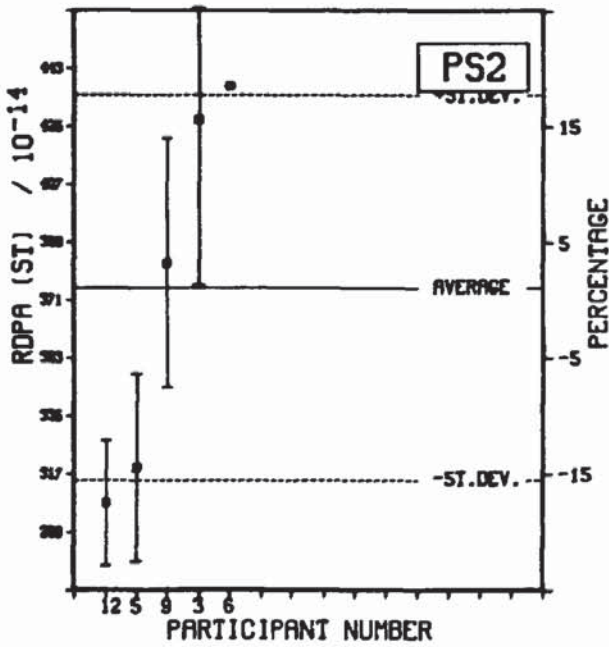
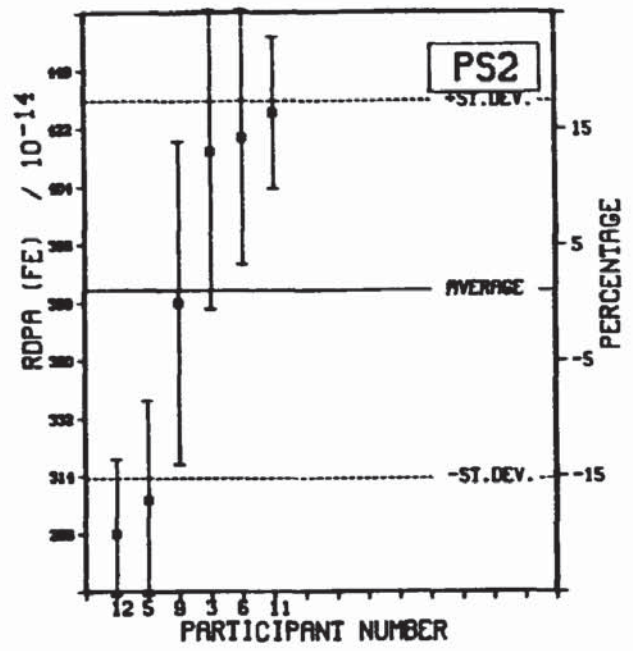
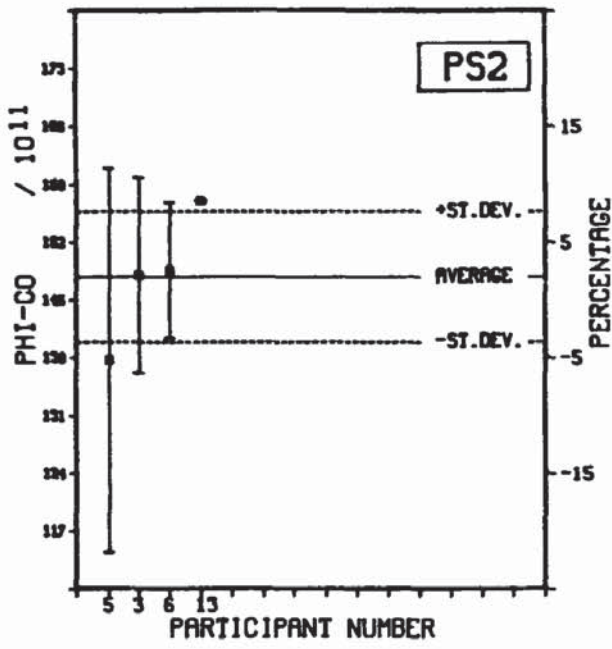


Fig. 7.c.2. PS2.

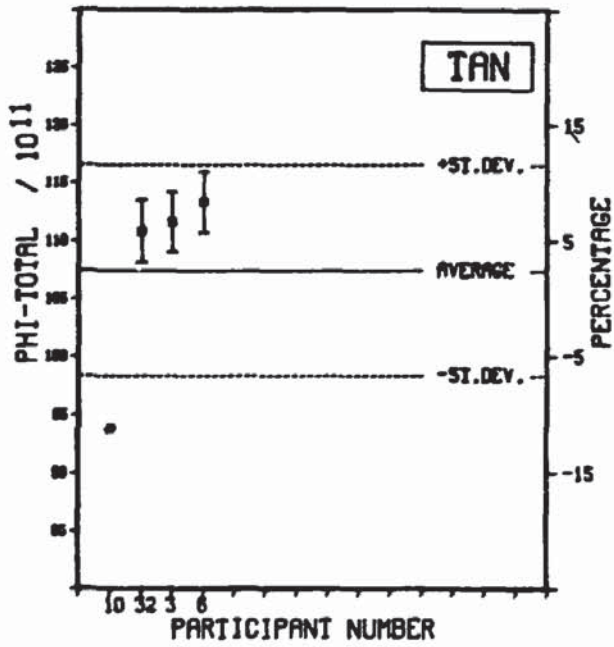
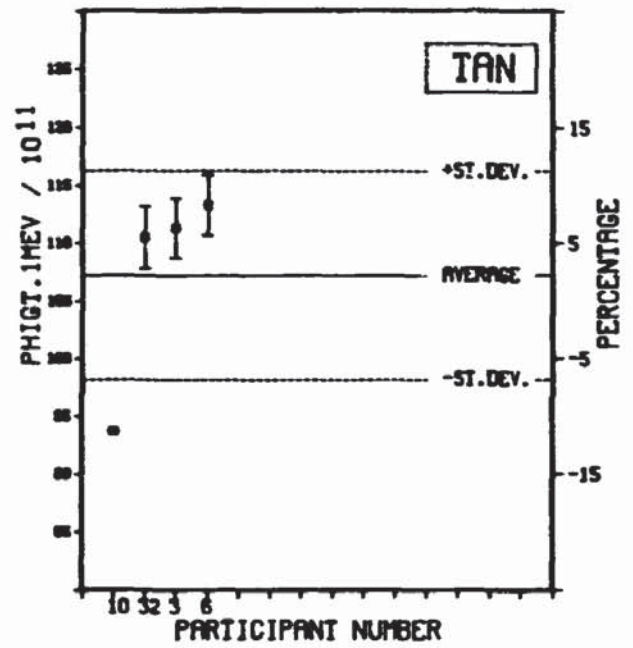
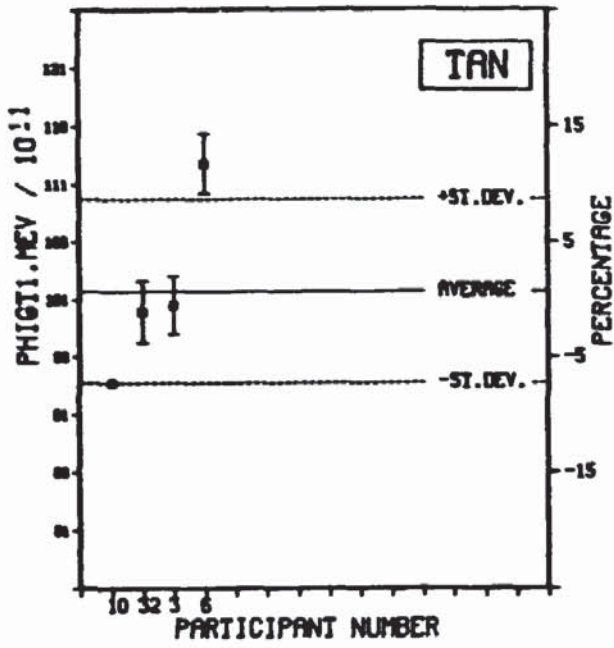


Fig. 7.d. TAN.

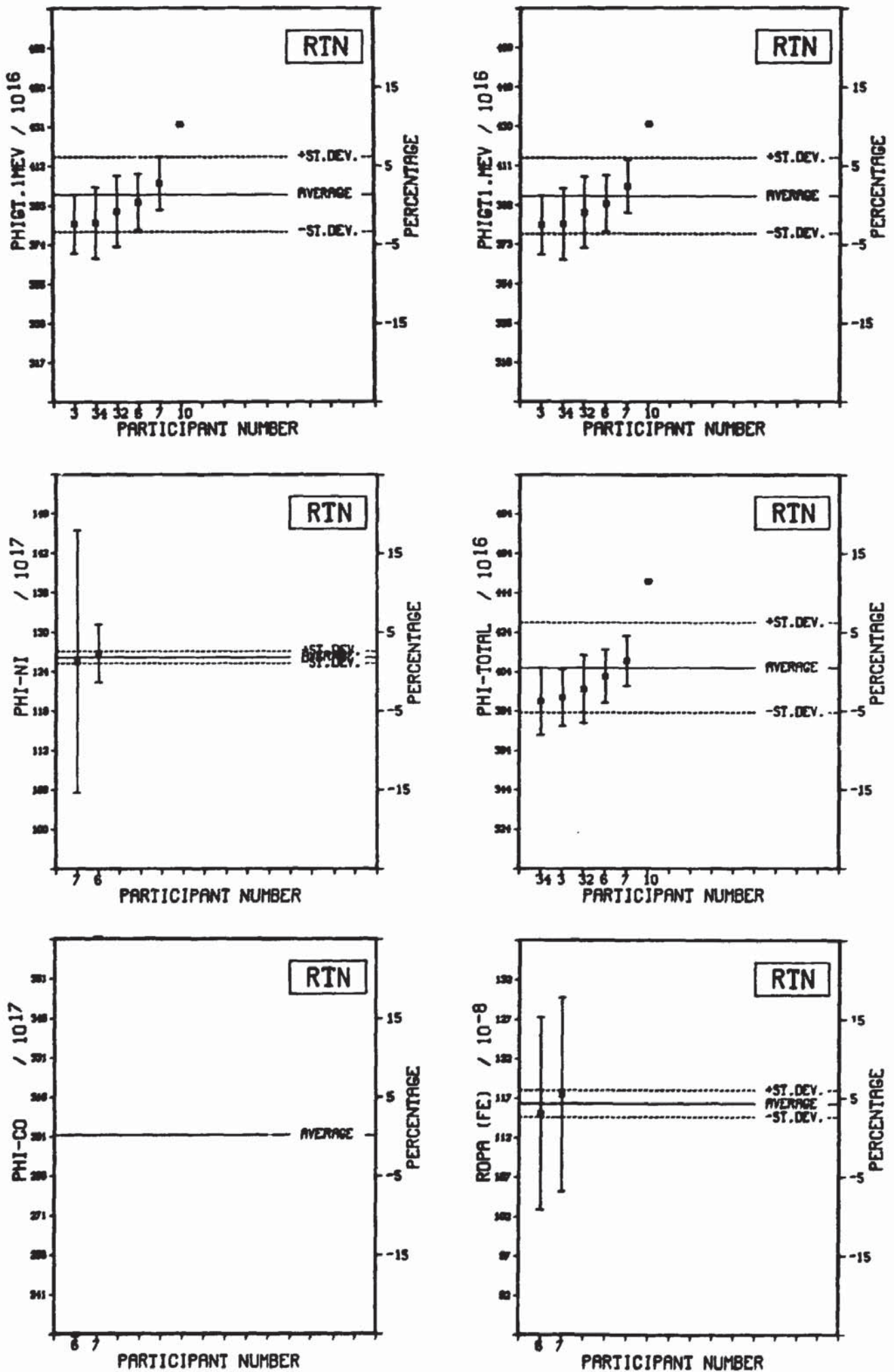


Fig. 7.e. RTN.

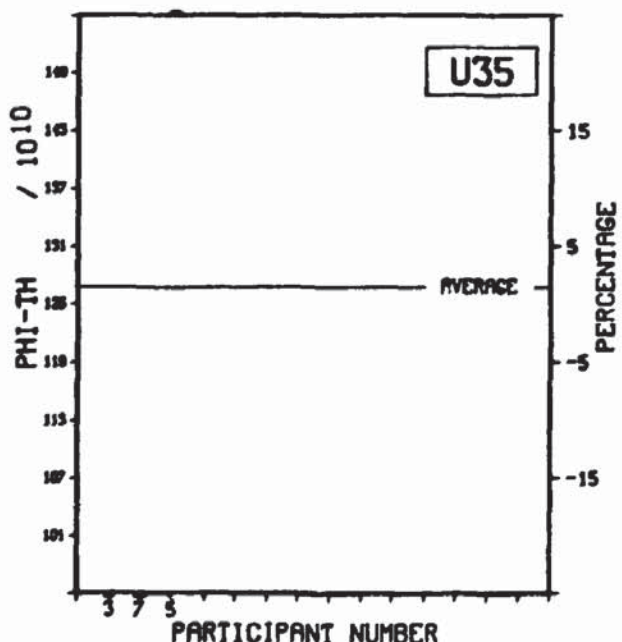
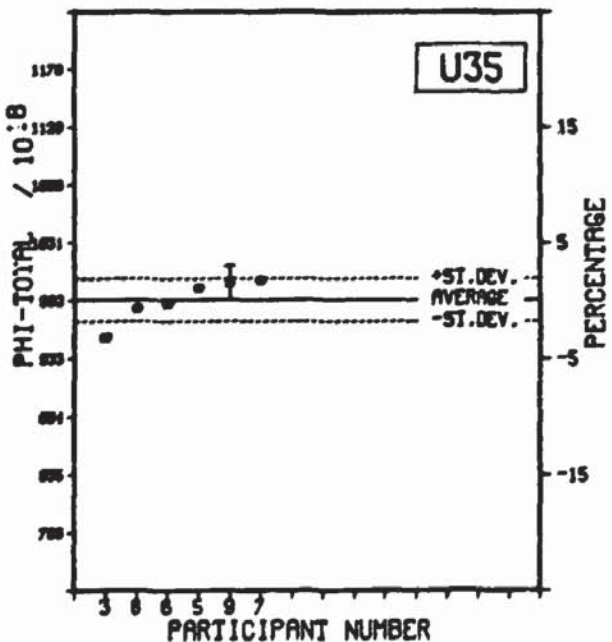
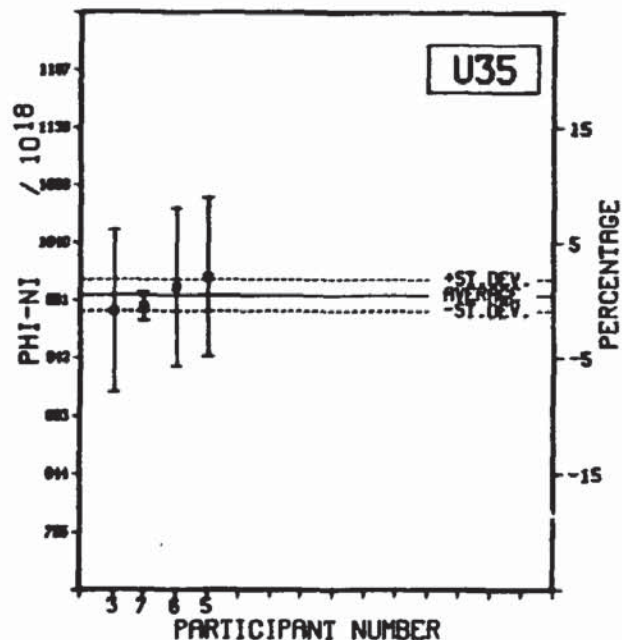
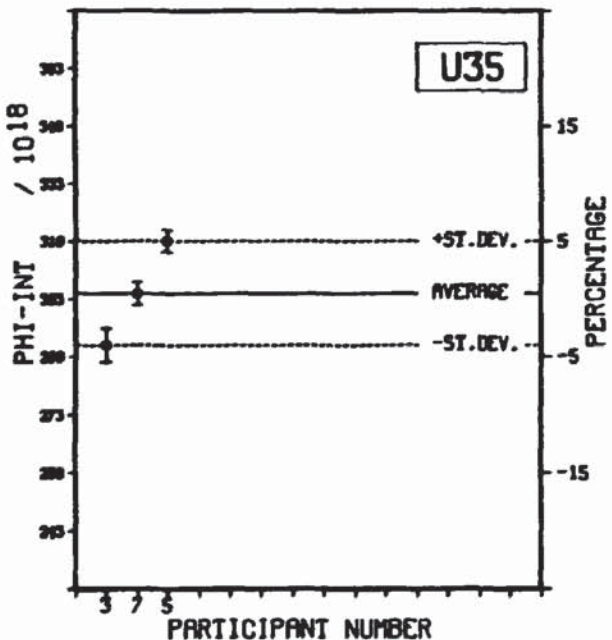
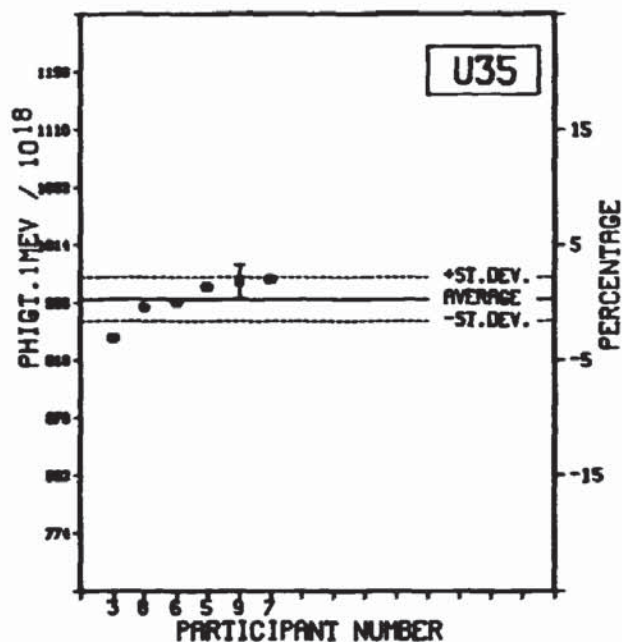
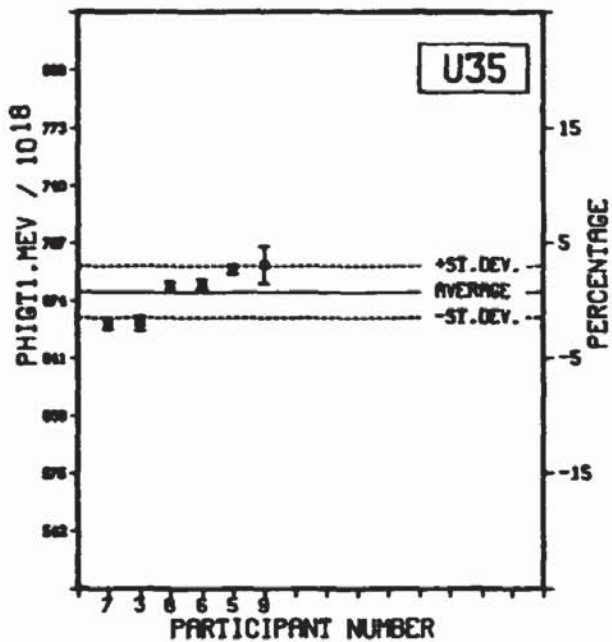


Fig. 7.f.1. U35.

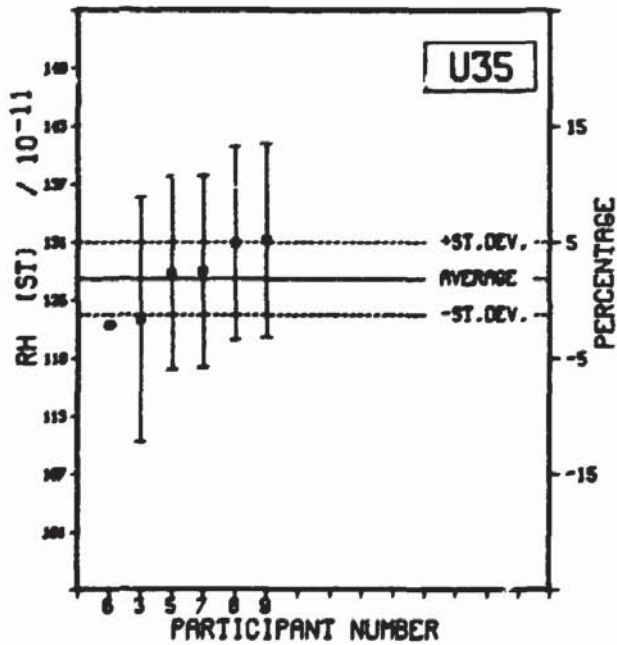
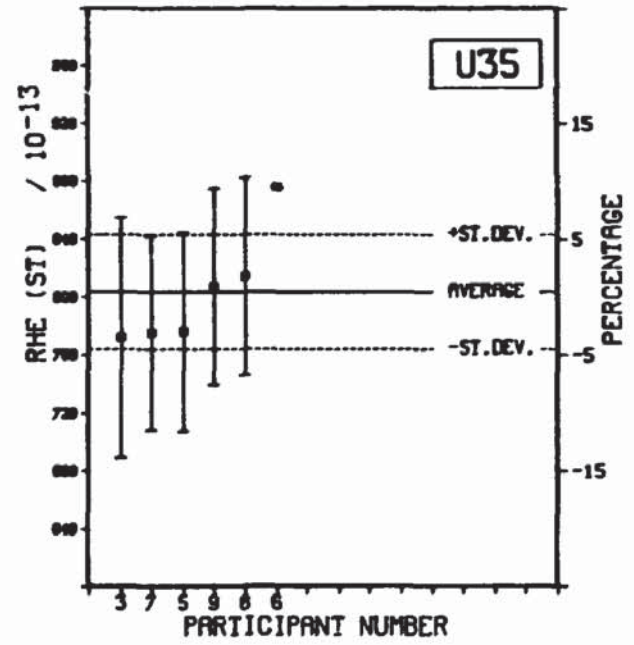
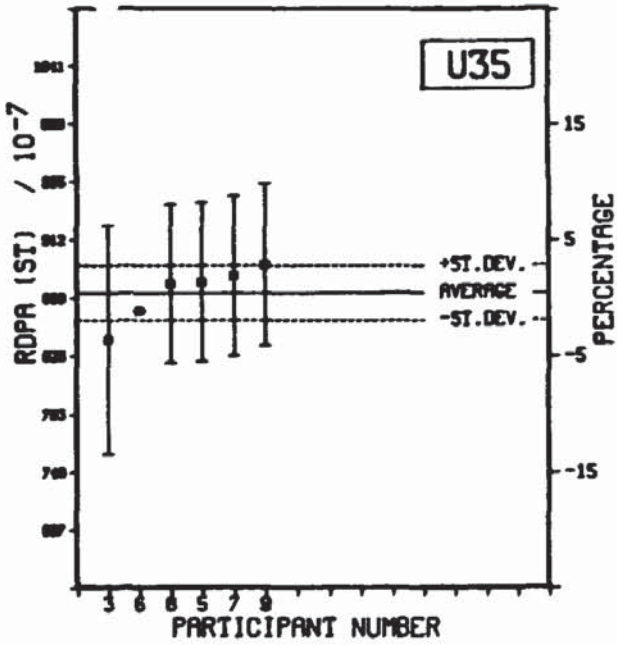
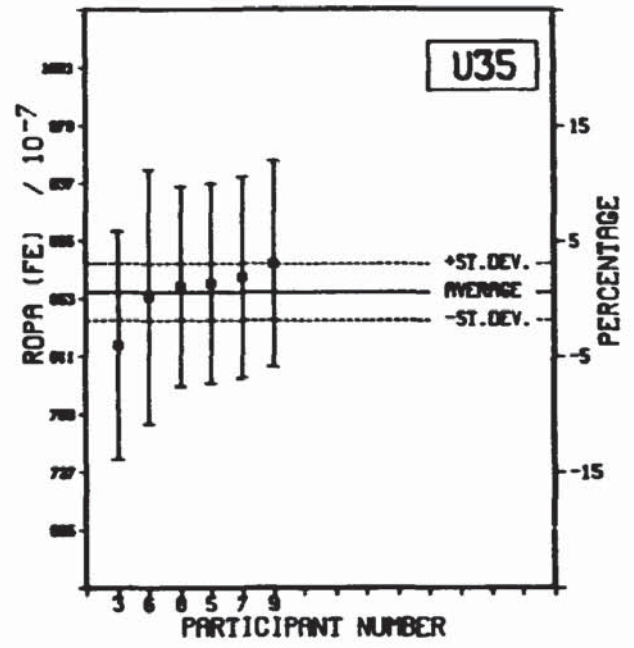
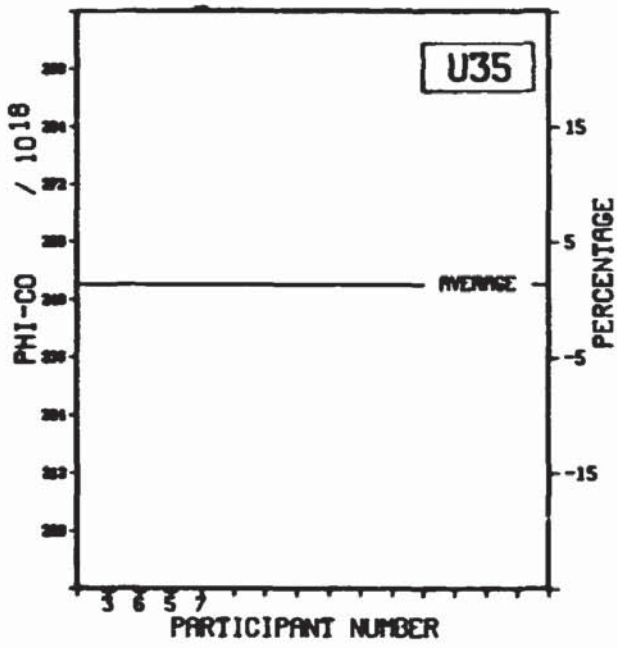


Fig. 7.f.2. U35.

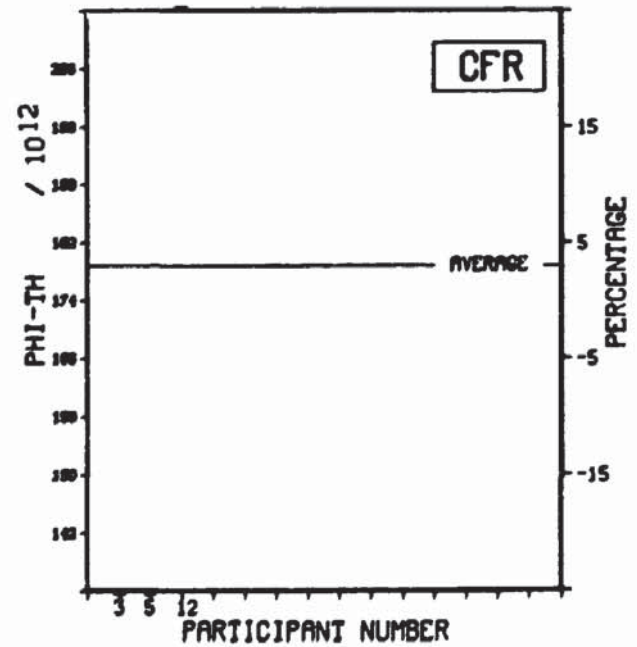
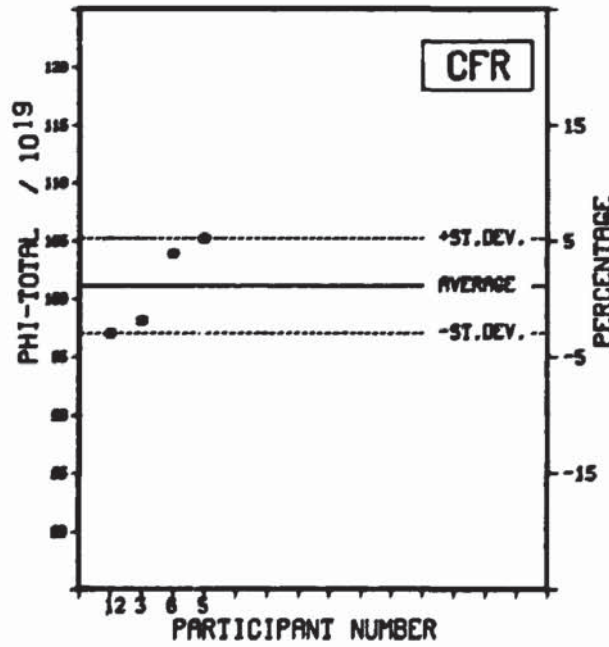
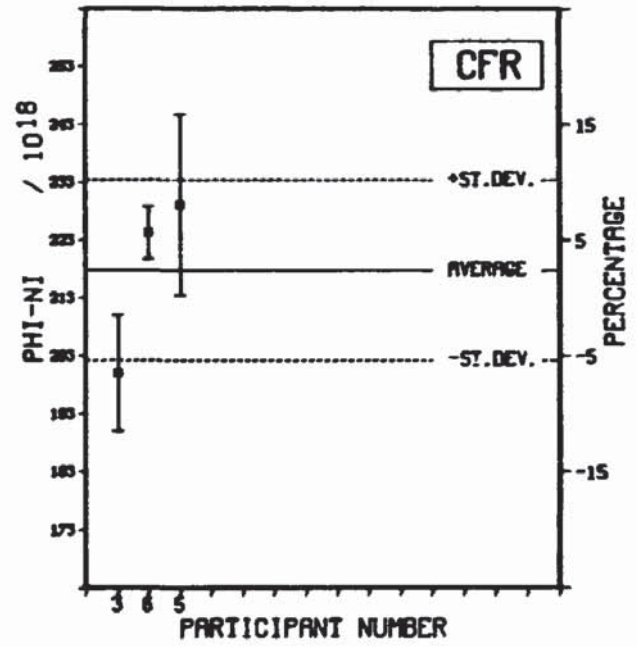
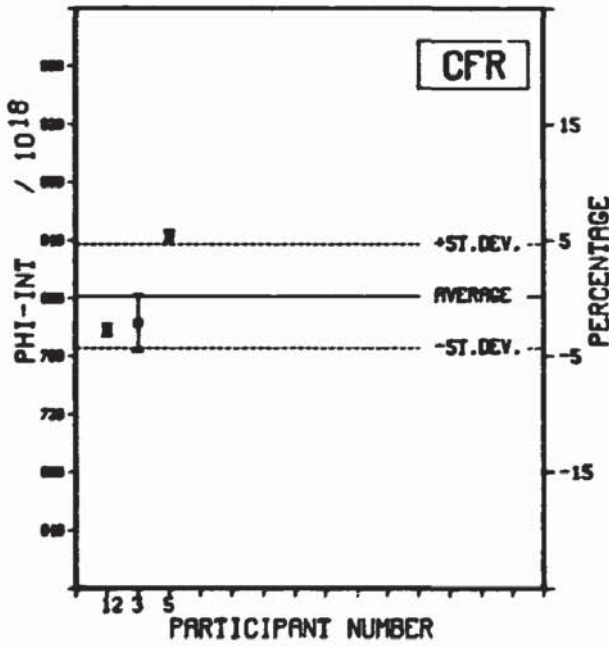
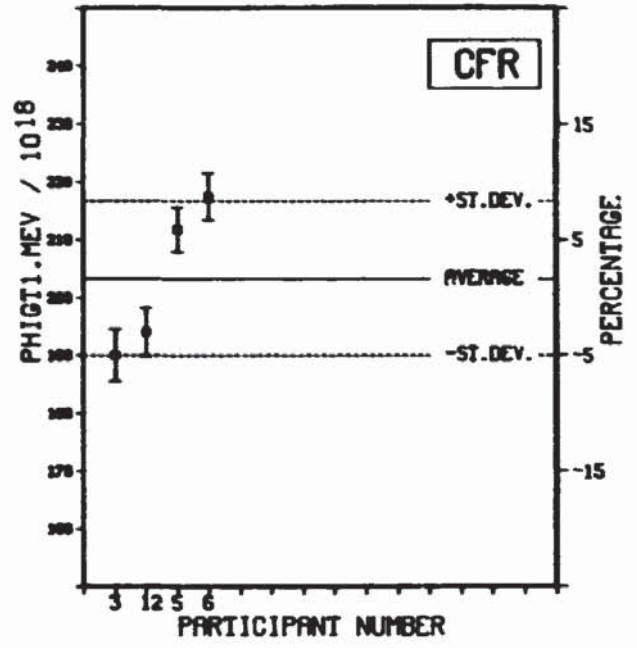
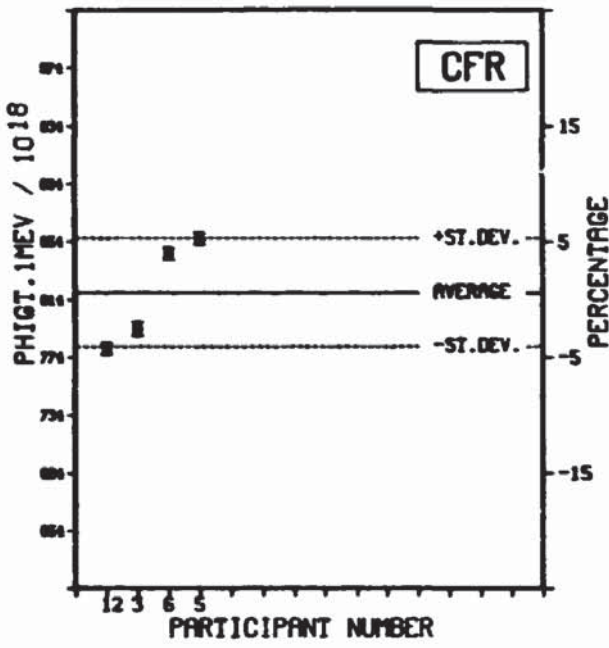


Fig. 7.g.1. CFR.

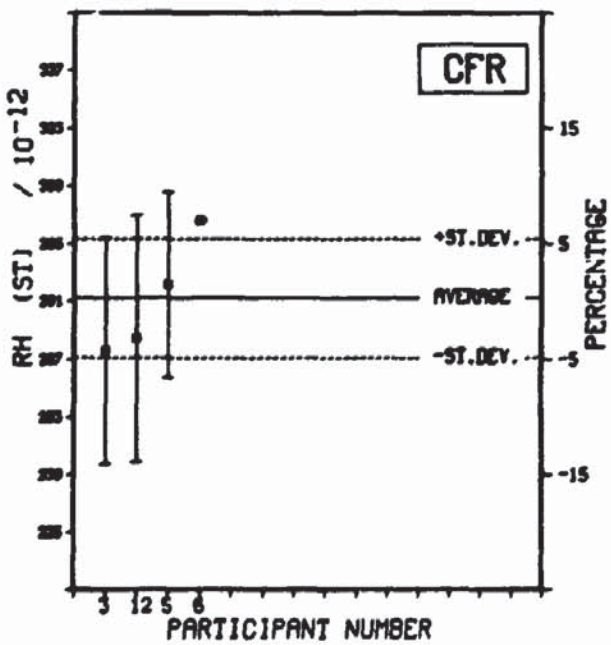
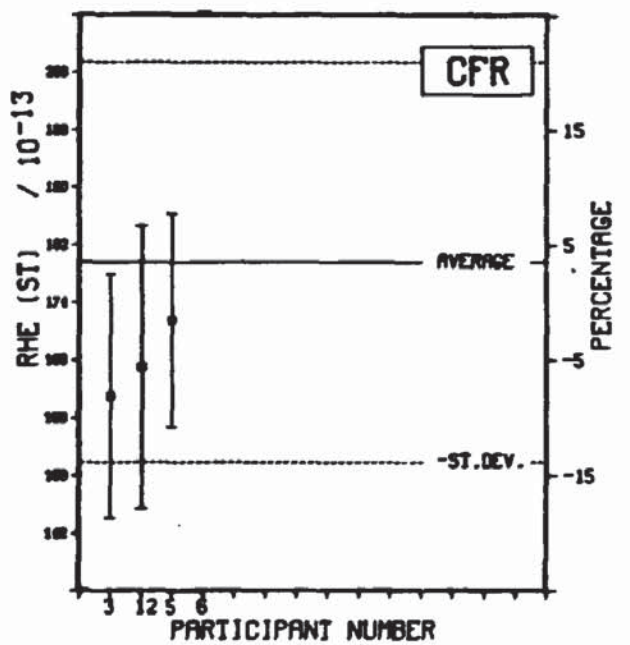
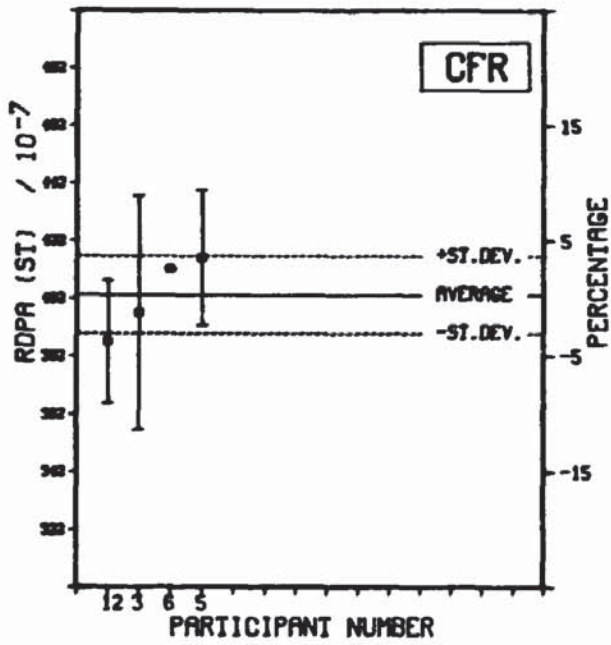
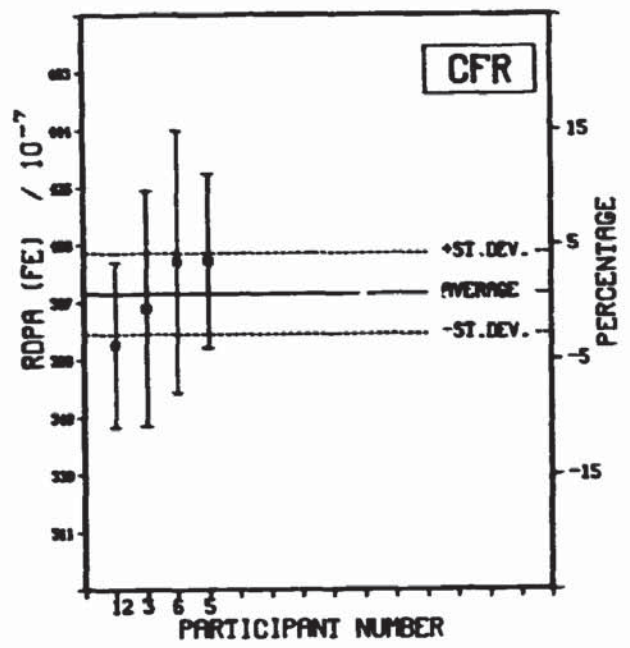
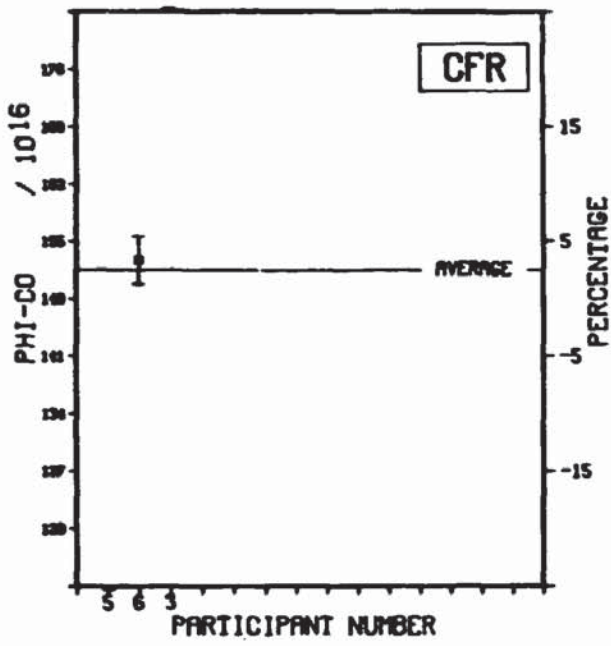


Fig. 7.g.2. CFR.

Appendix. Requirements of the covariance matrices used in the neutron spectrum adjustment.

(Part of this appendix is based on chapter 3 of [A1]).

The variables (the group fluence rate values, the measured reaction rates, and the group cross-section values) used in the neutron spectrum adjustment are assumed to obey a multivariate normal distribution in the linear space, owing to their evaluation method, i.e. the use of data originating from measurements. The normal character of the distribution is a consequence of the central-limit theorem.

The density of a normally distributed random variable x is

$$f(x) = \frac{1}{\sqrt{(2\pi)\sigma}} \exp \left[-\frac{1}{2} \left(\frac{x-x^*}{\sigma} \right)^2 \right]$$

satisfying the normalization condition

$$\int_{-\infty}^{\infty} f(x) dx = 1$$

where σ = standard deviation of x ;

x^* = expectation value of x .

Similarly, the general p -dimensional normal density function is written as

$$F(X) = (2\pi)^{-\frac{p}{2}} \cdot (\det(\Sigma))^{-\frac{1}{2}} \cdot \exp \left(-\frac{1}{2} (X-X^*)^T \Sigma^{-1} (X-X^*) \right) \quad (1)$$

satisfying the condition

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} f(X) dX_1 \dots dX_p = 1 \quad (2)$$

where X = vector containing the p random variables;

X^* = vector of expectation value of X ;

Σ = the covariance matrix of X .

The infinite integral (2) is equal to 1 if Σ is a positive definite symmetric matrix. The expression "positive definite" means that all the eigenvalues ("characteristic roots") of Σ are positive. (The elements of Σ may also be negative, of course).

The argument of the exponential function in (1)

$$-\frac{1}{2} (X-X^*)^T \Sigma^{-1} (X-X^*)$$

can be rewritten as

$$-\frac{1}{2} \chi^2$$

The value of χ^2 (chi-square) is often used for characterizing the consistency of the random sample X and the reference vector X^* . As the value of χ^2 decreases, the consistency increases due to the increase of $F(X)$:

$$F(X) = (2\pi)^{-\frac{1}{2}p} \cdot (\det(\Sigma))^{-\frac{1}{2}} \cdot \exp(-\frac{1}{2} \chi^2)$$

If r , the number of the positive eigenvalues of Σ , is smaller than the dimension p of the matrix and the remaining $(p-r)$ eigenvalues are zero, then Σ is positive semi-definite. (The rank of Σ is just r). In this case $F(X)$ is difficult to interpret since $\det(\Sigma)=0$.

However the covariance matrix can still be interpreted in a statistical sense, i.e. belonging to a singular density, in which the generalized inverse of the covariance matrix replaces the inverse of the matrix in formule (1).

It is noted that the $(p-r)$ variables of X can be expressed using the r independent variables, so the problem can be redefined in the r -dimensional sub-space of the p -dimensional space.

If the integration of formule (2) is performed over the correct hyperplane in the p -dimensional space, then the value of the integral is 1. There exists a direct relation between the mentioned singular distribution and a non-singular multivariate normal distribution in r dimensions.

(For further details see [A2]).

If one or more negative values are present in the set of eigenvalues of Σ , no suitable redefinition can be derived. (This may even happen if all the elements of the Σ matrix are positive). In this case the increasing difference between X and X^* in the directions of the eigenvectors belonging to the negative eigenvalues will decrease the χ^2 -value (moreover it can be negative (!) as well).

In cases, where the absolute values of the negative eigenvalues are small compared with the values of the positive ones, they may be substituted by zeros making the matrix Σ positive semi-definite.

In the next part the remarks are restricted to the positive definite matrices.

The numerical difficulties arising in the inversion of Σ are related to the condition number, that is the ratio of the largest eigenvalue to the smallest positive one. If the matrix is singular or nearly singular, then there occur stability problems in the process of matrix inversion. Then this matrix will be ill-conditioned; its determinant may be zero within computer accuracy and therefore it becomes positive semi-definite.

Another possibility for describing the situation is the use of the "effective rank" of Σ to characterize the degree of being ill-conditioned. (The effective rank of the matrix can be defined in several ways, see e.g. in [A3]). If the (effective) rank is less than the dimension of Σ , the same consequences are valid as written above.

Often a covariance matrix does not represent a final result, but is used as intermediate step in a numerical process for calculating other values. Then for instance a matrix $X^T X$ is formed from the data matrix X . The matrix $X^T X$ is much more sensitive to disturbances than the original matrix X . Special numerical methods exist to determine a solution starting from X instead of $X^T X$, in view to increase the stability of the problem.

Most of the numerical difficulties can be eliminated using the correlation matrices instead of the covariance matrices, i.e. by using the differences in the co-ordinates of X and X^* in "units of standard deviation" (see section 3.2 of [A3]).

The discussion given above describes the requirements of the covariance matrices from the point of view of mathematical statistics.

Finally, some notes from the point of view of physics:

- the covariance matrix of the neutron spectrum should have anti-correlated parts as well, due to its definition as described in [A4];
- the measured reaction rates are usually highly correlated, since the measuring/evaluating procedure contains a lot of common steps, so the expected correlation coefficients can lie in the range of 0.3-0.8 (see the data of the ANO reaction rates); a diagonal matrix in this case has no physical background (see also [A5]);
- more attention should be paid to the evaluation of the covariance matrices of the nuclear data, i.e. cross-sections and gamma-ray emission probabilities (gamma abundances) [A6].

References to appendix

- [A1] Morrison, D.F.: "Multivariate statistical methods", (McGraw-Hill, New York, 1978).
- [A2] Matzke, M.: "The covariance matrix of neutron spectra used in the REAL84 exercise", Report FMRB-108, (PTB, Braunschweig, August 1986).
- [A3] Zsolnay, É.M., and Nolthenius, H.J.: Proceedings of the IAEA Consultants' Meeting on the assessment of the results of the REAL84 exercise, Report INDC(NDS)-190/G+F+R, (IAEA, Vienna, March 1987).
- [A4] Szondi, E.J.: "The covariances matrix of neutron spectra", Report BME-TR-RES-10/86, (Nuclear Reactor of the Technical University, Budapest, January 1986).
- [A5] Szondi, E.J.: "An approximate method for developing the covariance matrix of a set of measured activities, Report BME-TR-RES-11/86, (Nuclear Reactor of the Technical University, Budapest, January 1986).
- [A6] Piksaikin, V. (ed): "Covariance methods and practices in the field of nuclear data", Proceedings of a IAEA specialists' meeting on Covariance Methods and Practices in the field of nuclear data held in Rome, Italy, 17-19 November 1986. Report INDC (NDS)-192 (IAEA, Vienna, January 1988).