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GENERATION OF COVARIANCE FILES FOR IRON-56 AND NATURAL IRON

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The Working Party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The Parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank Member countries), and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The following report was issued by a Subgroup investigating different methodologies to produce covariance data. These data are required to assess uncertainties in design parameters and to refine the use of nuclear data both in fission and fusion reactor applications. It was agreed to limit the scope to covariance data for Iron-56 and natural iron in view of their importance as structural materials in reactors and particularly for fusion reactor shielding applications.

The opinions expressed in this report are those of the authors only and do not represent the position of any Member country or international organisation. This report is published on the responsibility of the Secretary-General of the OECD.

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1. Work within the Subgroup

Considerable work has been done on most of the topics assigned to the Subgroup in the report on its initiation (NFA-FUS-90-03). In detail the following subjects have been addressed:

a) Sensitivity calculations especially for fusion reactor shielding problems – *Papers A 1-10*;

b) Generation of covariances for evaluated cross-sections of ^{56}Fe from model calculations by means of simple qualitative methods for cross-sections, elastic angular distributions and total gamma-production cross-sections – *Papers A 9-10, 23-25*;

c) Generation of covariances for ^{56}Fe cross-sections evaluated from model calculations and experimental data combined by least squares procedures – *Papers A 11-12*;

d) Detailed comparison of evaluated ^{56}Fe cross-sections and uncertainties derived by different methods with each other and with precise experimental data – *Papers A 11-13*;

e) Derivation of an accurate set of 14-MeV cross-sections for ^{56}Fe by quantitative evaluation of the experimental data base in order to provide a sensitive test for evaluated cross-sections and uncertainties – *Papers A 14-15*;

f) Work on proposals for formats for cross-section types not yet describable by ENDF/B format rules, such as coupled energy-angle distributions for secondary neutrons, and charged particle emission and total and energy-differential gamma-emission cross-sections – *Papers A 16-17*;

g) Derivation of cross-section covariances in the resonance range – *Paper A 26*;

In the course of this work among others the following results have been obtained:

a) Extensive sensitivity calculations have been performed for the shielding of the superconducting coils of a tokamak fusion reactor; and the sensitivity of the calculations to the different cross-section types and to the various energy ranges of each cross-section has been obtained in detail. Also the sensitivity of the shielding calculations to the P_1-P_3 coefficient of the elastic scattering distributions was investigated and proven to be important – *Papers A 1-7*.

b) The approximate methods for generation of covariances of cross-sections from model calculations used at ORNL and IRK have been documented – *Papers A 8-10* – compared with each other – *Paper A 13* –,with precision experimental data – *Papers A 14-15* – and with results from a more accurate evaluation – *Papers A 11-12*. From this comparison it can be concluded that the approximate methods for generation of covariances used in ENDF/B-VI and EFF have provided reliable uncertainty estimates and thus can be recommended for further use.

c) The method of estimating covariances from the dispersion of different evaluations has been extended from cross-sections (file 33 data) to elastic angular distributions, secondary energy distributions, and total and energy-differential gamma-production cross-sections – *Papers A 11-12*.

d) Two formats (MF 30 and 36) – *Papers A 16-17* – have been worked out in detail and proposed for proper dealing with covariances of coupled angle-energy distributions of secondary neutrons and charged particles, and total and energy-differential gamma-production cross-sections.

e) A new evaluation of all important cross-sections of ^{56}Fe has been performed using all available experimental information and combining it with the EFF-2 evaluation based model calculations using quantitative Bayesian methods – *Papers A 11-14*. It has been demonstrated that a large reduction of uncertainties (typically by factors 2-3) can be obtained in this way compared with evaluations completely based on model calculations. After two years this evaluation has been updated in 1994 by adding new accurate experimental data for a number of cross-

sections – *Paper A 22*. This has resulted in considerable further reduction of the cross-section uncertainties and – even more important – has fully confirmed the original evaluation within its stated uncertainties. Thus it appears that the approach developed in *Papers A 11-14* may be used generally for important materials in order to create accurate and easily updateable evaluations including reliable uncertainty information.

f) The problem of deriving covariances of cross-sections from nuclear model calculations from uncertainties of the model parameters was investigated in some detail. As yet, however, results tend to seriously underestimate the cross-section uncertainties – *Papers A 18-19*. This may be partly due to the use of too restricted parameter spaces and in part to the neglect of the inherent model deficiencies. More work on this – in principle promising method – is needed.

g) A complete set of covariances for the resonance parameters of ^{56}Fe was derived by F. Fröhner and put into ENDF format (file 32). There are, however, serious problems in the use of this information as the important potential scattering radii cannot at present be stored in the ENDF-6 format. Therefore also the existing codes neglect the uncertainties of the potential scattering radii and thus lead to unrealistically small cross-section uncertainties. In addition comparisons of cross-sections in the resonance range both between different recent experiments and with the reconstructions from the resonance parameters given in the most recent evaluations have revealed considerably larger discrepancies than expected from the estimated accuracies of both the data and the resonance parameters. Thus it appears that in file 32, uncertainties of the cross-sections in the resonance range need to be supplemented at present by file 33 information estimated by qualitative methods.

h) As a consequence of the work described in b-e), there exist now four evaluations, EFF-2.2, ENDF/B-VI, Vienna-Obninsk and CENDL-2 with complete file-33 information – *Paper A 8-12* – which have been compared in detail and found to agree within stated uncertainties.

i) As a result of the work for the new Vienna-Obninsk evaluation the experimental data base for ^{56}Fe has been compiled and thoroughly checked, and – unless given by authors – covariance matrices were estimated for each data set.

j) Most members of the Subgroup participated in the NSC Specialists' Meeting and Subgroup members acted as working group members and chairmen of this meeting. Thus the recommendations and conclusions of this meeting – *Paper A 20* – summarise to a large extent the conclusions of the Subgroup concerning generation and processing of covariances.

k) Based on the experience gained by the work within the Subgroup, H. Vonach, the co-ordinator, gave an overview at the Brookhaven meeting on *Evaluation Methodology – Paper A 21*.

2. Open problems

2.1 Representation of covariance information in the ENDF/B-VI format

The work of the Subgroup has demonstrated on the example of ^{56}Fe that the goal of generating reliable and rather complete covariance information can be obtained with reasonable effort. The actual use of this information, however, is today severely limited by the existing processing and sensitivity codes. At present only the information on cross-section covariances (file-33 data) and covariances of angular distributions for elastic and inelastic scattering to discrete levels (file-34 data) can be used in neutronics calculations. In order to also consider the effects of covariances of coupled energy-angle distributions of secondary neutrons, and total and energy-differential gamma-production cross-sections, considerable extensions of the present processing and sensitivity codes would be needed in order to handle the proposed new formats MF 30 and MF 36. Likewise the processing codes for transforming file-32 information (covariances of resonances) into covariances of group cross-sections have to be amended to include the covariances of all parameters especially those of the potential scattering radii. While this work is rather straightforward and should not pose major problems, it exceeds the resources available to the members of the Subgroup.

2.2 Covariances of calculated cross-sections

The problem of estimating the covariances of calculated cross-sections used so far – *Paper A 8-12* – is still rather crude and development of more rigorous methods is urgently needed. Attempts in this direction – *Papers A 18-19* – have shown that the consideration of the uncertainties of the model parameters is insufficient to explain the uncertainties of the theoretically calculated cross-sections and an explicit inclusion of the uncertainties due to the model

deficiencies is necessary for realistic uncertainties estimates. These, however, cannot be quantified easily. This is probably the most important, however, also most difficult open question concerning the generation of reliable covariance information of evaluated nuclear data.

Appendix A

Report of the initiation of Subgroup 2 on the generation covariance files for ^{56}Fe and natural Fe

H. Gruppelaar

1. Introduction

The NEANDC/NEACRP Working Group on International Evaluation Co-operation was founded at a joint session of NEANDC and NEACRP members at the NEACRP meeting in Argonne, October 9-13, 1989. A report is given in document NEACRP-A-1011/NEANDC-A-257. Six high-priority tasks were defined of which the first two are relevant to this paper:

1. Intercomparison of the files for Cr-52, Fe-56 and Ni-58,

2. Generation of covariance files for Fe-56 and natural Fe

For each task a Sub Working Group had to be initiated by D. Larson and H. Gruppelaar, respectively. This paper reports the progress in the initiation of Subgroup 2.

The task was described shortly as follows:

"Covariance data are required to assess uncertainties in design parameters (e.g., in the design of shields for the superconducting magnets of fusion reactors) and to refine the use of nuclear data in reactor applications. It is not always clear how much detail is required in the covariance files for different applications, the requirements being related to the sensitivity calculations. Collaboration in the general area of covariance files is beneficial to all parties. Initially it is proposed to concentrate on covariance data for Fe-56 and natural Fe in view of their importance in reactors, particularly for fusion shielding applications. The JEF-2/EFF-2 and ENDF/B-VI covariance data (files 32 and 33) should be intercompared and the methodology to produce these data should

be discussed. Possible improvements should be indicated. A study is also recommended of the methods used to evaluate and store covariance information for double-differential and photon production cross-sections."

I like to stress here that the proposed task has the rather wide purpose to improve the methods, to derive covariance files in general with special emphasis on Fe. Fe was chosen as an example to start with and to illustrate the various problems. It was also chosen to concentrate on one application and to avoid an open-ended activity. Still the participants should bear in mind that the final goal is to obtain methods to generate a general purpose file with covariance data for all materials.

2. Invitation to participate

After consultation with the chairmen of the various nuclear data projects in the OECD area, an invitation letter to participate in Subgroup 2 was sent out on December 18, 1989 to potential participants in Europe, Japan and the U.S.A. A copy was sent to the above-mentioned chairmen. This letter contained a proposal for a chairman (Dr. H. Vonach) and the following suggestions for activities:

2.1. Sensitivity studies. Which data are most important?

a. energy and angle-integrated cross-sections
b. energy distributions
c. angular distributions
d. coupled energy-angle distributions

These studies depend on the applications, e.g., the shielding of superconducting magnets in a fusion reactor

2.2. Exchange of information on codes and methods for sensitivity calculations

2.3. Exchange of information on methods for the evaluation of covariance data

a. from experimental data
b. from theory and uncertainties in model parameters
c. from a combination of experimental data and models.

2.4. Exchange of information on formats and how to use these formats in practical applications

2.5. Simple methods to generate covariance files

2.6. Inspection of previous results with regard to covariance data for Fe. Comparison of (preliminary) EFF-2/JEF-2, JENDL-3 and ENDF/B-VI files and (as far as available) covariance files

2.7. Evaluation of covariance data for cross-sections in broad energy ranges (stored in file 33)

2.8. Evaluation of covariance data for resolved resonances, or only for important resolved resonance

2.9. Evaluation of covariance data for energy-angle distributions

2.10. Evaluation of covariance data for photon production

2.11. Evaluation of covariance data for the natural element

2.12. Evaluation of covariance data for group constants and transfer matricies

It was asked to indicate which topics were of most interest to the potential members and also, to mention possible other items and ideas for a working plan and time-schedule. Also any material relevant to these points was requested for general distribution: Annexes of the invitation letter, including mailing lists and NEACRP-A-1011.

3. Received answers

Most scientists invited to Subgroup 2 have reacted in a positive way. Some have not explicitly answered, but it may be assumed that those listed in Section 4 will actively participate. There may be further interest from the users' side and from the non-OECD region. A name that has been suggested is Prof. Dr. Zhou Deling (CNDC, P.R. China). All invited scientists agreed with the choice of Prof. Vonach as a chairman of Subgroup 2.

It is noted that the present task is also of interest to the community of dosimetry users. However, the emphasis of Subgroup 2 is more directed to general purposes. Nevertheless, contacts with colleagues working in the dosimetry field are recommended. This is already guaranteed by the participation of some members of the group.

The received reactions are summarised below.

3.1. NEA Data Bank/ NNDC/ RSIC/ Subgroup 1

Some very useful assistance could be given by the NEA Data Bank in relation to graphical intercomparisons or recent evaluations for iron (Dr. C. Nordborg) and the provision of (utility and sensitivity) codes and derived (covariance) libraries (Dr. E. Sartori). Similar services could be performed by NNDC (Dr C. Dunford). With respect to shielding sensitivity and covariance codes the RSIC could also play an important role. Furthermore, with respect to the possibility to derive some information on uncertainties from the dispersion between different data files, it is important to keep in good contact with the chairman of Subgroup 1 (contact Dr. D. Larson).

3.2. Europe (EFF/JEF)

Positive reactions were obtained from Dr. H. Vonach (IRK-Vienna), Dr. F. Fröhner (KfK) and Dr. J. Kopecky (ECN-Petten). A new name was also suggested: Dr. A. Hogenbirk from ECN-Petten.

Furthermore, there is considerable interest in applications of covariance data to shielding problems: e.g., at the NET team in Garching, at PSI-Würenlingen, at CEA-Saclay (Mr. I. Kodeli; see his contribution on PWR shielding to the Marseille PHYSOR-90 meeting), at CEA-Cadarache (Dr. M.A. Santamarina) and ECN-Petten (Dr. A. Hogenbirk, who is performing sensitivity and covariance calculations for the NET shielding). Contact with these users is recommended.

All invited participants are involved in the EFF-2 project (coordinator: Dr. Gruppelaar). The main emphasis of this project has recently been redirected to the calculation of a shielding data base for the NET fusion reactor, including covariance data. The strategy of EFF-2 with respect to covariance data is as follows:

a. Determine sensitivities of NET shielding parameters to cross-sections. Include studies with respect to energy and angular distributions (SED and SAD).

b. Use presently available methods and data to make a first estimate of the uncertainties in the shielding parameters.

c. Improve covariance data base with priorities taken from studies a.,b. Some approximate methods could be used initially (i.e., only file 33 and approximate methods for SED/SAD).

Drs. Fröhner and Kopecky are involved in the JEF-2 project (chairman: Dr. Salvatores as well). The EFF-2 and JEF-2 projects are closely linked together; a common meeting is scheduled at the NEA Data Bank in the last week of May 1990

Dr. Vonach is specialised in the high-energy range (above 1 MeV) and has considerable experience in covariance evaluation for the international dosimetry file. Dr. Fröhner is an expert in the resolved resonance region. Dr. J. Kopecky and Dr. A. Hogenbirk are involved in the EFF-2 project and are currently working on the formatting of the evaluations for structural materials both for JEF-2 and EFF-2. The high-energy range of the EFF-2 evaluations for the major isotopes of Fe, Cr and Ni are contributed by Prof. M. Uhl (IRK, Vienna).

The present status of JEF-2 with respect to Fe is that the-file (only for isotopic data) is ready for benchmark testing. The EFF-2 file for Fe will be equal to JEF-2 except for the energy part of Fe-56 above 1 MeV, which has been evaluated by Dr. M. Uhl. The EFF-2 file for Fe is assembled at ECN, Petten and will be ready before summer 1990. (covariance files for Fe will be constructed by simple means as soon as possible, starting with diagonal covariances for the most important reactions and for the strongest S-wave resonances.

3.3. Japan

Three names have been suggested from the JENDL project by Dr. Kikuchi. Two scientists from JAERI were mentioned: Dr. A. Hasegawa (Shielding laboratory) and Dr M. Sugimoto (LINAC laboratory) and Prof. Y. Kanda from Kyushu University. At present JENDL-3 does not yet contain covariance data. As this is considered for the near future, there is considerable interest to study methods for implementing these data.

Dr. Kanda has specified to be interested in topics 2.3, 2.6 and 2.8, mentioned in Section 2. A discussion with regard to topic 2.3 – *Exchange on information on methods to evaluate covariance data* – is given in a contribution of Y. Kanda and Y. Uenohara to the Mito conference (1988) – p. 1041 of the proceedings "Covariance matrices evaluated by different methods for some neutron-dosimetry reactions". Prof. Kanda intends to estimate covariances for some reactions of Fe by applying the methods mentioned in this reference and then intercomparing his results and comparing them with those from other evaluations. He is also interested to see the developments in assigning covariances to resolved resonances. He stresses that also the data files should be intercompared (Subgroup 1).

The status of JENDL-3 for Fe is that it has been released in Japan for benchmark testing. There are no covariance data included as yet.

3.4. U.S.A.

Dr. C.Y. Fu has written that he is interested in the co-operation on this task force. From a recent summary of the November 1989 Cross-Section Evaluation Working Group (CSEWG) meeting (distributed on February 1, 1990), two names for Subgroup 2 were proposed:

Dr. C.Y. Fu and Dr. D. Hetrick, both from Oak Ridge National Laboratory. It may be of interest to note that both are also participating in Subgroup 1.

Some preliminary covariance data for the structural materials were already presented at the afore-mentioned CSEWG meeting. They consisted of diagonal uncertainties for most reactions in file 3 of ENDF/B-VI. Some ideas to create these files were presented. To represent the resolved resonance region, it is possible to assign errors to the "background" cross-section in file 3, even if this cross-section is zero. Thus, for a fast and preliminary evaluation of errors only file 33 is necessary. The inclusion of correlations is complicated because the covariance matrices should be positive definite. This can be accomplished by using the LB=8 law, but it is questioned whether the use of this law might introduce artificial features into the covariance matrices. Thus, further work is necessary on this item.

The checking and processing capabilities for files 32 and 33 are in a good shape (latest versions of BNL checking codes and NJOY). For file MF=30 these possibilities are lacking (also for MF=34,35?). The advanced options of MF=30 could be used to represent covariances by means of sensitivities and covariances of parameters which represent the compiled data. This could be a future option to represent uncertainties in double-differential data (MF6).

The next CSEWG meeting takes place in May 1990. Several Subgroup 2 members will participate. Dr. Vonach will also be present. At that meeting more news about the covariance file of Fe has to be expected.

The status of ENDF/B-VI for Fe is that the file will be released very soon, probably with some covariance data. Otherwise the file will be released without covariance data and further testing of the covariance data follows.

4. Establishment of Subgroup 2

From the above-mentioned reactions it is clear that there is interest and enthusiasm to establish Subgroup 2 with the following members:

Prof. Dr. Y. Kanda (Kyushu University)
Dr. A. Hasegawa (JAERI)
Dr. M. Sugimoto (JAERI)

Dr. C.Y. Fu (ORNL)
Dr. D. Hetrick (ORNL)

Prof. Dr. H. Vonach (IRK, Vienna; chairman)
Dr. F. Fröhner (KfK, Karlsruhe)
Dr. J. Kopecky / Dr. A. Hogenbirk (ECN, Petten)

The initiator of Subgroup 2 has sent a letter containing this report to these members. Starting from May 1, 1990 the working group has been established and Dr. Vonach will co-ordinate the further activities. My task will be to monitor the progress and to report the progress to the Working Group on International Evaluation Co-operation.

Important progress should be communicated to the following persons:

Dr. C. Nordborg / Dr. E. Sartori (NEA Data Bank)
Dr. Y. Kikuchi (JAERI)
Dr. M. Salvatores (CEA, Cadarache)
Dr. C.L. Dunford (BNL, Brookhaven)
Dr. H. Gruppelaar (ECN, Petten)

4. Programme of Subgroup 2

A programme to start the work of Subgroup 2 has been discussed at an ad-hoc meeting in Petten on April 9, 10 with Drs. H. Vonach, J. Kopecky, A. Hogenbirk and K.A. Verschuur. It is based upon the suggestions of Sections 2 and 3 and the opinions of the participants of the above-mentioned ad-hoc meeting.

The programme contains four elements:

A. Investigation why covariance data are important and how the user applies these data to real problems.

This includes essentially items 2.1. and 2.2.

4.1. Sensitivity studies. Which data are most important?

a. energy and angle-integrated cross-sections
b. energy distributions
c. angular distributions
d. coupled energy-angle distributions

These studies depend on the applications, e.g., the shielding of superconducting magnets in a fusion reactor or shielding problems of a PWR. Dosimetry problems should not be emphasised in this study.

4.2. Exchange of information on methods and codes for sensitivity calculations

Point 4.1 is performed at Petten (Hogenbirk). Interesting results show, that for the inboard shielding, the energy range below a few hundred keV are unimportant in contrast to the 14 MeV elastic and inelastic cross-sections. A paper on this subject is being prepared. There are also results forthcoming from I. Kodeli (CEA-Saclay) on PWR shielding.

Point 4.2 could be an action for the NDB and RSIC. Codes that could be used are SENSIT and SUSD. Further developments may be necessary, in particular for SED/SAD treatment.

B. Investigation of methods and formats to produce covariance data

This includes items 2.3, 2.4, 2.5.

4.3. Exchange of information on methods for the evaluation of covariance data

a. from experimental data
b. from theory and uncertainties in model parameters
c. from a combination of experimental data and models

4.4. Exchange of information on formats and how to use these formats for practical applications (files 30-35)

4.5. Simple methods to generate covariance files, e.g., to obtain immediate results or to obtain results that can be processed and used immediately

Existing literature should be compiled and scanned. Format information should come from CSEWG, LANL, BNL, ORNL, etc.

There are problems with LB8 and uncertainties about MF30, MF34, MF35. Can the processing codes treat advanced options? Do the users know how to use these advanced options? Are there sensitivity/covariance codes to treat these options? (NDB, RSIC)

There is interest from Drs. Vonach and Kanda to work on problems 4.3 and 4.5. A very simple method is to derive uncertainty information from inter-comparison of new evaluations, see next point.

C. Comparison of existing data and covariances

This includes item 2.6, which is also part of Subgroup 1.

4.6. Inspection of previous results with regard to covariance data for Fe. Comparison of (preliminary) EFF-2/JEF-2, JENDL-3 and ENDF/B-VI files and (as far as available) covariance files

Following the work of Subgroup 1 (with priority for Fe!) useful uncertainty information can be derived from the spread in the data. Distribution of the new files is of high priority. Also graphical intercomparisons are desired. (NDB, BNL, JAERI).

Dr. Vonach would like to use this information.

There is also some information from existing covariance data, e.g., COVFILS (ENDF/B-V) and the work of the NEA Data Bank and perhaps soon the preliminary covariance data from ENDF/B-VI. These data could be inspected or reviewed (distr. NDB, BNL, RSIC). Participation in the review of ENDF/B-VI could be a good suggestion. At Petten the NDB covariance data are used to perform test calculations of the uncertainty in NET shielding calculations. Further work with preliminary data if available is considered.

A good plotting option for covariance data is required (NJOY, BNL?). Probably the NJOY code contains or will contain these features.

In view of the importance of 14 MeV data for fusion reactor applications a re-evaluation of experimental 14 MeV data could be considered (H Vonach).

D. Construction of covariance data for each file

This includes items 2.7 to 2.12.

4.7. Evaluation of covariance data for cross-sections in broad energy ranges (stored in file 33)

4.8. Evaluation of covariance data for resolved resonances, or only for important resolved resonances

4.9. Evaluation of covariance data for energy-angle distributions

4.10. Evaluation of covariance data for photon-production

4.11. Evaluation of covariance data for the natural element

4.12. Evaluation of covariance data for group constants and transfer matrices

This is an action for all three parties.

The easiest way is to start with point 4.7, also for the resolved range. For fusion application the high-energy range is clearly very important.

The next priority could be point 4.8, starting with the most important S-wave resonances (Fröhner, etc.).

Point 4.9 is too complex at present and should be simplified.

First the uncertainty in the elastic angular distributions should be investigated. It is not yet clear how important this is and how this should be dealt with. A simple solution is to evaluate the uncertainty in the P1 term.

The evaluation of uncertainties in secondary energy distributions is another problem. Sensitivity codes can use the "median" approach. If this is effective it is simple, but there is now a way to store this information in ENDF format.

New developments are necessary to store energy-angle correlated covariance data and uncertainties in photon production spectra (4.10). This may be possible with MF30 in the near future. With respect to point 4.11 one should think about the problems related with the fact that Fe-56 is only one isotope of the natural element. A simple solution is to assume that the uncertainties for Fe-56 are representative for natural Fe. The evaluation of covariance data for group constants and transfer matrices could be done with the processing code (NJOY), only as far as the information is available on the basic files. If this is not practical (perhaps in the case of SED/SAD) other input should be given to the users' codes (e g. uncertainty in the median in the case SENSIT is used). This could be a practical solution now (use of code ANGELO for change of group structure), but is not attractive on the long run.

E. Intercomparison of covariance data for Fe-56

Finally, the three (new) covariance data should be compared and some calculations of applications should be made.

5. Time schedule

It is rather difficult to give a detailed time schedule at present. An optimistic time schedule is to finish the work for A and B within one year and to have at least some covariance files for Fe-56 ready as well. After about one year the programme should be re-evaluated and new priorities should be set.

Appendix B

List of documents originating from the work of Subgroup 2

1) A. Hogenbirk
"Self-Shielding in the Net Fusion Reactor Blanket and Effects of Uncertainty Calculations", Report ECN-R-90-007 (1990).

2) A. Hogenbirk, H. Gruppelaar and K.A. Verchunv
"Sensitivity and Uncertainty Analysis of Net/ITER Shielding Blankets", Report ECN-RX-90-062 (1990).

3) A. Hogenbirk
"Sensitivity and Uncertainty Analysis of the Nuclear Heating in the Coils of a Fusion Reactor", Report ECN-RX-90-34 (1990).

4) A. Hogenbirk
"Energy Self-Shielding and SED/SAD Effects in Sensitivity Calculations of a Net Shielding Blanket", Report ECN-RX-91-038 (1991).

5) A. Hogenbirk
"Extensive Sensitivity/Uncertainty Analysis of a Net Fusion Reactor Blanket", EFF-DOC-128 (1991).

6) A. Santamarina and T. Parish
"Uncertainty Analysis of the Net/ITER S.C. Coil Shielding Parameters to Cross Section Data Uncertainties", Contribution *to International Workshop on Fusion Neutronics, June 5, 1992, Los Angeles, U.S.A.*

7) A. Hogenbirk
"New Sources of Uncertainties in Sensitivity/Uncertainty Studies", *Proceedings of the 17th Symposium on Fusion Technology, September 14-18, 1992, Rome, Italy*.

8) A. Hogenbirk
"Uncertainty Calculations Made Easier", Contribution to *8th International Conference on Radiation Shielding, April 24-28, 1994, Arlington, Texas, U.S.A.*, Report ECN-RX-94-035.

9) A. Hogenbirk
"Calculation of Design Uncertainties for the Development of Fusion Reactor Blankets Taking into Account Uncertainties in Nuclear Data", Contribution *to Int. Conf. on Nuclear Data for Science and Technology, May 9-13 1994, Gatlinburg, Tennessee, U.S.A.*

10) A. Hogenbirk
"Extensive Neutronic Sensitivity/Uncertainty Analysis of a Fusion Reactor Shielding Blanket", *Fusion Engineering and Design* **24** (1994) 275-286.

11) T. Parish and A. Santamarina
"Sensitivity and Uncertainty Analysis of the Net Magnet Neutronic Design Parameters to Uncertainties in Cross Section Data" (pre-print).

12) H. Vonach et al.
"Uncertainty Estimates for the Fast Neutron Cross Sections for the European Fusion File EFF-2 for ^{52}Cr, ^{56}Fe, ^{58}Ni and ^{60}Ni", EFF-DOC.85 (1990).

13) S. Tagesen and H. Vonach
"Uncertainty Estimates for the EFF-files for ^{52}Cr, ^{56}Fe, ^{58}Ni and ^{60}Ni", *Proc. Int. Conf. on Nuclear Data for Science and Technology, Jülich, Germany, May 12-17, 1991*, Springer Berlin Ed. S. Qaim, p. 871.

14) D.M. Hetrick, D.C. Larson and C.Y. Fu
"Generation of Covariance Files for the Isotopes of Cr, Fe, Ni, Ca and Pb in ENDF/B-VI", Report ORNL/TM-11763 Oak Ridge (1991).

15) H. Vonach et al.
"Evaluations of the Fast Neutron Cross Sections of ^{56}Fe including Complete Covariance Information", *Physics Data* **13-7** Fachinformationszentrum Karlsruhe (1992).

16) V. Pronyaev et al.
"Updating of a Theoretical Evaluation by Experimental Data in the Case of ^{56}Fe", *Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data, October 7-9 1992, Oak Ridge, U.S.A.*, NEA/NSC/DOC(93)3 p.135.

17) S. Tagesen and D.C. Larson
"Approximate Methods for Derivation of Covariance Data",
Proc. International Symposium on Evaluation Methodology, October 12-16 1992, Brookhaven, U.S.A. (in press).

18) H. Vonach et al.
"Evaluation of 14 MeV Cross Sections for the Main Isotopes of the Structural Materials Fe, Cr and Ni", *Proc. Int. Conf. on Nuclear Data for Science and Technology", Jülich, May 12-17, 1991*, Springer Berlin Ed. S. Qaim, p. 906.

19) A. Pavlik et al.
"Evaluation of 14 MeV Cross Sections for the Main Isotopes of the Structural Materials Cr, Fe and Ni", *Physics Data* **13-6**, Fachinformationszentrum Karlsruhe (1991).

20) D.W. Muir
"Description of Covariances of Emission Spectra using ENDF File 30", *Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data, 7-9 Oct. 1992, Oak Ridge, U.S.A.*, NEA/NSC/DOC(93)3 p.195.

21) H. Vonach
"Direct Covariance Data for Coupled Energy-angle Distributions", *Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data, 7-9 Oct. 1992, Oak Ridge, U.S.A.*, NEA/NSC/DOC(93)3 p.183.

22) Y. Kanda
"Generation of Covariance Data from Combined Experimental and Theoretical Data", *Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data, 7-9 Oct. 1992, Oak Ridge, U.S.A.*, NEA/NSC/DOC(93)3 p.119

23) T. Kawano et al.
"Estimation of Nuclear Reaction Model Parameters for ^{59}Co, ^{58}Ni and 60Ni. *Proc.Int.Conf. on Nuclear Data for Science and Technology, May 12-17, 1991, Jülich, Germany,* , Springer Berlin Ed. S. Qaim, p. 974.

24) Report of Working Group A "Generation of Covariances to meet User Needs" and,
Report of Working Group B "Covariance File Formats and Processing" *Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data, 7-9 Oct. 1992, Oak Ridge, U.S.A.*, NEA/NSC/DOC(93)3 p. 289.

25) H. Vonach
"Covariances of Evaluated Nuclear Data - Present Status and prospects for the Future", *Proc. International Symposium on Evaluation Methodology, 12.-16. October 1992, Brookhaven, U.S.A.* (in press).

26) V.G. Pronyaev, S. Tagesen and H. Vonach
Update and Improvement of the IRK Evaluation for ^{56}Fe, *Proc. Int. Conf. on Nuclear Data for Science and Technology, May 9-13 1994, Gatlinburg, U.S.A.* (in press).

27) Zhao Zhixiang and Lin Tong
"Uncertainty Files for Neutron Cross Sections and Elastic Angular Distributions on ^{56}Fe", EFF-DOC-266 (1993).

28) Lin Tingjin et al.
"Intercomparison of Fe, Cr, Ni Neutron Data from CENDL-2, BROND-2 and ENDF/B-VI and JENDL-3", *Proc. Int. Conf. on Nuclear Data for Science and Technology, May 9-13 1994, Gatlinburg, U.S.A.* (in press).

29) Zhao Xiang et al.
"Evaluation of Neutron Induced Data on ^{56}Fe", *Comm. Nucl. Data Progress*, Vol. 11, 56 (1994).

30) F. Fröhner
"On Uncertainty Evaluation and Fluctuations in the resolved and unresolved Resonance Regions", *Proc. Int. Conf. on Nuclear Data for Science and Technology, May 9-13 1994, Gatlinburg, U.S.A.* (in press).

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