



INDEX

1 - INTRODUCTION	p. 4
1.1 - Background	p. 5
1.2 - JEFF-3.1/3.1.1 Evaluated Nuclear Data Library	p. 8
1.3 - Cross Section Processing and Testing	p. 9
2 - LIBRARY SPECIFICATIONS	p. 10
2.1 - Name	p. 11
2.2 - Materials, Temperatures and Background Cross Sections	p. 12
2.3 - Energy Group Structure	p. 23
2.4 - Weighting Function	p. 31
2.5 - Legendre Order of Scattering	p. 37
2.6 - Convergence Parameters	p. 37
2.7 - Processing Codes and Procedures	p. 37
2.8 - Response Functions	p. 41
3 - LIBRARY VALIDATION	p. 48
3.1 - Reactor Physics Benchmarks	p. 48
3.2 - Shielding Benchmarks	p. 49
4 - CONCLUSION	p. 56
REFERENCES	p. 58
APPENDIX A - Samples of NJOY and SMILER Input Listings for a Standard Nuclide	p. 64
Sample of NJOY Input for Generating the Neutron GENDF File for a Standard Nuclide	p. 65
Sample of NJOY Input for Generating the Photon GENDF File for a Standard Nuclide	p. 68
Sample of SMILER Input for Converting a Standard Nuclide File from the GENDF Format to the AMPX Master Format	p. 69
APPENDIX B - Samples of NJOY and SMILER Input Listings for a Bound Nuclide	p. 70
Sample of NJOY Input for Generating the Neutron GENDF File for a Bound Nuclide	p. 71

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	3	75

Sample of NJOY Input for Generating the Photon GENDF File for a Bound Nuclide p. 74

Sample of SMILER Input for Converting a Bound Nuclide File from the GENDF Format to the AMPX Master Format p. 75

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	4	75

VITJEFF311.BOLIB - A JEFF-3.1.1 Multi-Group Coupled (199 n + 42 γ) Cross Section Library in AMPX Format for Nuclear Fission Applications

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1 - INTRODUCTION

The ENEA-Bologna Nuclear Data Group produced a multi-group coupled neutron and photon cross section library in AMPX format for nuclear fission applications, based on the OECD-NEA Data Bank JEFF-3.1.1 /1/ (see also /2/ and /3/) evaluated nuclear data library. For this purpose, cooperation was established with a former specialist of the State Scientific Center of the Russian Federation Institute for Physics and Power Engineering of Obninsk (SSC RF IPPE-Obninsk). The result of this effort is the present VITJEFF311.BOLIB library, which has the same neutron and photon energy group structures (199 neutron groups + 42 photon groups) and general basic features as the DLC-184/VITAMIN-B6 /4/ American library in AMPX format, based on the ENDF/B-VI Release 3 /5/ American evaluated nuclear data library. The generation of the present library took into account the experience accumulated by the ENEA-Bologna Nuclear Data Group in the data processing and testing of the previously generated VITJEF22.BOLIB /6/ and VITJEFF31.BOLIB /7/ similar libraries in AMPX format, respectively based on the JEF-2.2 /8/ and JEFF-3.1 /2/ OECD-NEA Data Bank evaluated nuclear data libraries. The production of the VITJEFF311.BOLIB library intends to propose to the users of the JEFF-3.1.1 nuclear data a VITAMIN-B6-type library, i.e., a fine-group pseudo-problem-independent cross section library based on the Bondarenko /9/ (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects. For “pseudo-problem-independent multi-group library” is understood that the library is prepared with enough detail in energy, temperatures and neutron resonance self-shielding so as to be applicable to a wide range of physical systems.

The VITJEFF311.BOLIB library was generated through an updated automatic calculation procedure based on the LANL NJOY-99.259 /10/ nuclear data processing system, with the updating “upnea049”, and the ENEA-Bologna 2007 Revision /11/ of the ORNL SCAMPI /12/ nuclear data processing system. In particular this automatic procedure, developed at the ENEA-Bologna Nuclear Data Group, permits to produce quickly large group-wise cross section libraries in AMPX format with the potential of generating, through further proper data processing with the ENEA-Bologna 2007 Revision of the SCAMPI system, broad-group working libraries of collapsed and self-shielded cross sections in AMPX or FIDO-ANISN format for different applications. Concerning this, the ENEA-Bologna Nuclear Data Group generated recently the BUGJEFF311.BOLIB /13/ broad-group coupled neutron and photon working cross section library in FIDO-ANISN /14/ format, through problem-dependent cross section collapsing of the VITJEFF311.BOLIB library. In particular the BUGJEFF311.BOLIB library adopts the neutron and photon energy group structures (47 neutron groups + 20 photon

groups) of the ORNL DLC-0185/BUGLE-96 /4/ similar library derived from VITAMIN-B6 and it is dedicated to LWR shielding and pressure vessel dosimetry applications.

Finally, the VITJEFF311.BOLIB library was extensively tested on many thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments.

1.1 - Background

In recent years, the multi-dimensional deterministic transport codes using group-wise cross section libraries extended their practical simulation capability to an enlarged variety of nuclear systems, characterized by different neutron spectra and high geometrical complexity. In particular the three-dimensional (3D) discrete ordinates (S_N) codes like, for example, TORT /15/ /16/, increased their competitiveness with respect to the corresponding 3D Monte Carlo stochastic codes, as for example MCNP /17/. Comparable or even more convenient performances in terms of CPU times were in fact obtained with the same calculation precision, similar description capability of complex geometries and suitable simulation of different neutron and photon spectral conditions. Various factors concurred, in particular, to determine the increased flexibility and convenience in the practical use of the 3D discrete ordinates codes: the impressive increased performance of modern computers, innovative general-purpose fine-group cross section libraries with upscatter cross sections and new ancillary pre/post-processor systems of programs, dedicated to simplify and to strengthen the preparation and the graphical verification of the input of the geometrical model.

About the availability of innovative fine-group libraries, for example, the interesting features of the VITAMIN-B6 /4/ library must be underlined. Unlike similar previous libraries as VITAMIN-C /18/, VITAMIN-E /19/ or VITAMIN-J /20/, VITAMIN-B6 introduced fine-group discretization (more than 30 neutron groups) in the thermal neutron energy region below about 5 eV, including upscatter cross sections. This has the potential of treating with precision, together with the present fast calculation performances, problems where a rigorous description of the thermal neutron spectrum is essential. This is specifically requested, for example, in the case of the boron neutron capture therapy (BNCT) medical applications /21/ or when it is necessary to calculate (see /22/) the thermal neutron and photon radiation damage, as emerged for some material testing reactors (MTRs) /23/ and light water reactors (LWRs) /24/ /25/. The ENEA-Bologna Nuclear Data Group contributed, in particular, in this sector with the following libraries, freely distributed by OECD-NEA Data Bank: VITJEF22.BOLIB /6/ and VITJEFF31.BOLIB /7/ in AMPX format together with MATJEF22.BOLIB /26/ and MATJEFF31.BOLIB /27/ in MATXS format. VITJEF22.BOLIB and MATJEF22.BOLIB are based (see also /28/), in particular, on the JEF-2.2 /8/ OECD-NEA Data Bank evaluated nuclear data library while VITJEFF31.BOLIB and MATJEFF31.BOLIB (see also /29/) are respectively based on the JEFF-3.1 /2/ OECD-NEA Data Bank evaluated nuclear data library (VITJEFF31.BOLIB) and on both the JEFF-3.1 and JEFF-3.1.1 /1/ evaluated nuclear data libraries (MATJEFF31.BOLIB).

At present, the availability of the VITJEFF311.BOLIB library permits to obtain derived working libraries of collapsed and self-shielded cross sections, through the ENEA-Bologna 2007 Revision /11/ of the SCAMPI /12/ data processing system. More specifically, the cross sections can be collapsed by the MALOCS module, can be self-shielded by the BONAMI module and finally can be converted into the AMPX or the FIDO-ANISN /14/ format. The

cross sections in AMPX format can be used by the XSDRNPM one-dimensional (1D) discrete ordinates transport code, included in the SCAMPI data processing system. The cross sections in FIDO-ANISN format can be used by the discrete ordinates transport codes included in the following US packages of deterministic codes: the ORNL DOORS-3.2 /16/ system (including the ANISN-ORNL 1D code, the DORT 2D code and the TORT 3D code), the LANL PARTISN-5.97 /30/ 3D parallel system and the ATTILA /31/ 3D commercial code with unstructured spatial grids (finite elements). Moreover the cross sections in FIDO-ANISN format can be read by the discrete ordinates transport codes of the Russian package CNCSN 2009 /32/, including the ROZ-6.6 1D code, the KASKAD-S-2.5 (serial) and KASKAD-S-3.0 (parallel multi-threaded) 2D codes and the KATRIN-2.0 (serial) and KATRIN-2.5 (parallel multi-threaded) 3D codes. Finally the cross sections in FIDO-ANISN format are used by the ORNL MORSE /33/ 3D Monte Carlo code.

Concerning the possibility to describe very complicated geometries requiring 3D spatial analyses, it is underlined that, up to recent times, only 3D Monte Carlo codes could obtain satisfactory results with high calculation precision. At present, with the recent introduction and availability of new pre/post-processor systems (e.g., the ENEA-Bologna BOT3P /34/ /35/ /36/ /37/ and the Japanese TORTWARE /38/ systems) of ancillary programs dedicated to the multi-dimensional deterministic transport codes for the automatic generation and graphical verification of the spatial mesh grids of the geometrical model, the simulation capability of complex geometries with the multi-dimensional discrete ordinates transport codes increased dramatically. This induced, obviously, an increased interest to give more options in terms of updated and flexible group-wise cross section library availability. The performance of the three-dimensional discrete ordinates transport codes can be now highly competitive with that of the 3D Monte Carlo codes.

About the cited pre-post-processor ancillary programs, the ENEA-Bologna Nuclear Data Group originally developed the BOT3P system (distributed by OECD-NEA Data Bank and ORNL-RSICC), which was extensively tested on neutron shielding benchmark integral experiment calculations /39/ /40/ /41/ /42/ /43/ with the DORT 2D and TORT 3D codes. The BOT3P system, based on combinatorial geometry algorithms, was initially dedicated to the DORT and TORT discrete ordinates transport codes of the DOORS system but it is now easily possible to generate automatically detailed spatial mesh grids also for any other possible transport code (through simple interfaces dedicated to manage the BOT3P binary output files), together with the graphical verification of the input data of the geometrical model.

Two meaningful applications confirmed, in particular, the flexibility and the performance of BOT3P supporting the DORT and TORT codes: 2D and 3D analyses /44/ in Cartesian geometry of PWR fuel assemblies, with a very fine approximated description of the cylindrical fuel pins and heavy 3D (about 2.0×10^6 spatial cells) fixed source calculations /45/ in cylindrical geometry, addressed to obtain the heating rate distribution in the internals of a large Westinghouse AP1000 pressurized water reactor (PWR).

Concerning the deterministic codes, it is really an upsetting fact that the 3D deterministic transport codes currently cannot be fully used for the scarce free availability (see /13/ and /46/) of broad-group working libraries also when their use should be strongly recommended and, in any case, competitive with the use of the 3D Monte Carlo stochastic codes. It is interesting to note that the industrial organizations presently continue to be interested in the

use /45/ or even in the development /47/ of the 3D deterministic codes. Moreover they directly generate /48/, for example, or outsource to external nuclear data processing working groups, under specific contracts, the broad-group working cross section libraries for radiation shielding and radiation damage calculations with the deterministic transport codes. In fact they must fulfil quality assurance procedures with respect to the nuclear safety authority requirements and when deterministic codes are employed there is no need, as in the case of the Monte Carlo codes, to justify the validity of the statistics adopted since the deterministic codes are based on rigorous analytical solutions of the neutral particle transport equations. It is underlined, in particular, that the 3D deterministic codes applied, for example, to radiation shielding and radiation damage analyses assure, with only a single run, a simultaneous and accurate average dose determination in every spatial position of the reactor geometrical model. It is then very important to underline that the deterministic transport codes permit reliable and effective sensitivity and uncertainty analyses, particularly recommended in the data validation activity and in a modern and rigorous approach to the industrial project of a nuclear reactor.

Taking into account the previous notes, it is considered important (see /46/), in general, to update and to extend further the availability of the fine-group multi-purpose cross section libraries dedicated to the simulations of nuclear fission systems with discrete ordinates codes. As already mentioned, starting from these libraries, derived broad-group working cross section libraries can be generated with parameterized sets of collapsed and self-shielded cross sections for the various applications, characterized by specific compositional, geometrical, spectral and temperature conditions. It is underlined that the generation of broad-group working libraries contributes to give, in particular, a strong impulse to promote the use of the 3D discrete ordinates transport codes, like TORT, which could have convergence problems when fine-group working libraries are used with hundreds of thousands of volumetric spatial meshes, possibly needed to describe accurately complex in-core and ex-core reactor geometrical models.

In particular, an increased generation of broad-group working libraries like BUGJEFF311.BOLIB /13/, derived from fine-group multi-purpose libraries like VITJEFF311.BOLIB, would permit to extend the field of application of the modern multi-dimensional discrete ordinates deterministic codes which can continue to offer important complementary information /22/ /39/ /40/ /41/ /42/ /43/ /44/ /45/ /49/ with respect to the results obtained with the Monte Carlo codes.

Moreover, since deterministic transport codes are going to be employed in the analysis of the Generation IV nuclear reactor projects within the European Union research activities, it would be highly recommended /46/ that a specific interest dedicated to the generation of broad-group working cross section libraries should be promoted.

It is expected, in particular, that the multi-purpose nature of VITJEFF311.BOLIB, like the VITAMIN-B6 library, will make this library useful for shielding and, potentially, for reactor physics analyses with JEFF-3.1.1 /1/ nuclear data.

In conclusion, during the last years, the ENEA-Bologna Nuclear Data Group has performed several actions addressed to generate practical tools to increase, in particular, the performance and competitiveness of the 2D and 3D deterministic transport codes, following the recommendations proposed by the OECD-NEA Data Bank.

1. Several fine-group cross section libraries /6/ /7/ /26/ /27/ /28/ /29/ and broad-group working cross section libraries /13/ /50/ for nuclear fission applications were generated and are presently freely distributed by OECD-NEA Data Bank and/or ORNL-RSICC.
2. A pre/post-processor system /34/ /35/ /36/ /37/ of programs for the automatic spatial mesh generation, dedicated to the 2D and 3D deterministic transport codes, was developed and it is now freely distributed by OECD-NEA Data Bank and ORNL-RSICC.
3. Transport analyses dedicated to fission reactor neutron shielding benchmark experiments /39/ /40/ /41/ /42/ /43/ /50/ were performed also within the activities /39/ of the OECD-NEA Nuclear Science Committee TFRDD Task Force /22/ on nuclear fission reactor ageing problems.
4. The whole set of the IRDF-2002 /51/ dosimetry cross sections was processed /52/ in the 47 neutron group structure of the BUGLE-96 /4/ cross section library using a flat neutron spectrum and neutron weighting spectra calculated with JEFF-3.1.1 and ENDF/B-VII.0 /53/ data, at one quarter of the thickness of a typical PWR pressure vessel: these data are partially included in the package of the BUGJEFF311.BOLIB /13/ library

1.2 - JEFF-3.1/3.1.1 Evaluated Nuclear Data Library

The VITJEFF311.BOLIB fine-group mother library from which the BUGJEFF311.BOLIB /13/ library was generated, is based on the JEFF-3.1.1 /1/ evaluated nuclear data library which was released at the end of February 2009. With respect to the previous version JEFF-3.1 /2/, it contains a total of 23 modified evaluated data files: updated evaluated files for twelve isotopes (O-16, Zr-91, Zr-93, Zr-96, Tc-99, Ru-103, Cs-135, Pm-147, Pm-148g, Eu-154, Np-237 and Pu-239) and corrected evaluated files for eleven isotopes (Cl-35, Ca-46, Cr-52, Fe-56, Mo-95, Rh-103, I-127, I-129, Ir-191, Ir-193, U-233).

For the next release, JEFF-3.2, more efforts on fission product evaluations, minor actinide evaluations and inclusion of more covariance data in the files are foreseen.

The other evaluated files of JEFF-3.1.1 are identical to those of the JEFF-3.1 evaluated nuclear data library, a version of the JEFF (Joint Evaluated Fission and Fusion) nuclear data file, released by the OECD-NEA Data Bank in May 2005. The JEFF project is a collaborative effort among the member countries of the OECD-NEA Data Bank to develop a reference nuclear data library. The JEFF library contains sets of evaluated nuclear data, mainly for fission and fusion applications; it contains a number of different data types, including neutron and proton interaction data, radioactive decay data, fission yield data, thermal scattering law data and photo-atomic interaction data.

While the objective of the previous JEF-2.2 library (1992) /8/ was to achieve improved performance for existing reactors and fuel cycles, its successor, the JEFF-3 project aims at providing users with a more extensive set of data for a wider range of applications. While existing reactors and fuel cycles remain the essential application areas of the nuclear data library, innovative reactor concepts (Generation-IV systems), transmutation of radioactive waste, fusion, medical applications and various non-energy related industrial applications are now also envisaged as scientific application areas that will make the use of the JEFF data.

Extensive benchmarking of the JEFF-3.1 data library was performed for both the general-purpose and the special-purpose sub-libraries. The official report (“The JEFF-3.1 Nuclear Data Library”, OECD-NEA Data Bank, JEFF Report 21, 2006 /2/) presents only results from

extensive benchmarking effort on criticality, effective delayed neutron parameters and shielding using a Monte Carlo approach (MCNP /17/ code). A wider validation of benchmark results using different methods (deterministic and Monte Carlo codes) for various integral quantities was promoted. The validation effort dedicated to the JEFF-3.1.1 updated and corrected data files for the 23 isotopes previously cited is described in “The JEFF-3.1.1 Nuclear Data Library”, OECD-NEA Data Bank, JEFF Report 22 /1/.

The content of the JEFF-3.1/3.1.1 evaluated nuclear data libraries is the following. The neutron general purpose library contains incident neutron data for 381 materials from H-1 to Fm-255. The activation library (based on the European Activation File, EAF-2003) contains 774 different targets from H-1 to Fm-257. The radioactive decay data library contains data for 3852 isotopes, of which 226 are stable. The proton special-purpose library contains incident proton data for 26 materials from Ca-40 to Bi-209. The thermal scattering law library covers 9 materials and the fission yield library covers 19 isotopes of neutron induced fission yield from Th-232 to Cm-245 and 3 isotopes with spontaneous fission yields (Cm-242, Cm-244 and Cf-252).

Concerning, in particular, the general purpose data library, new evaluations are included in JEFF-3.1 for the Ti isotopes (IRK-Vienna), the Ca, Sc, Fe, Ge, Pb and Bi isotopes (NRG-Petten), Rh-103, I-127, I-129, the Hf isotopes, U-236, U-237, U-238 and Am-241. For other isotopes more recent evaluations from other libraries were adopted.

Revised thermal scattering data have been produced for all important moderator and structural materials and this was included in JEFF-3.1 and remained unchanged in JEFF-3.1.1. The thermal scattering law library contains the following nine evaluations: hydrogen bound in water, hydrogen bound in zirconium hydride, hydrogen bound in polyethylene (CH₂) and CaH₂, deuterium bound in D₂O, Be-9, graphite, Mg-24 and finally calcium bound in CaH₂. All the cited data files are new evaluations, except Be-9 and hydrogen in polyethylene, which are from the JEFF-3.0 /54/ library (April 2002). Many of the evaluations are the result of an IAEA co-ordinated project on thermal neutron scattering. Calculations for a variety of temperatures were made with the LEAPR module of the NJOY /10/ nuclear data processing system to obtain thermal scattering data that are accurate over a wider range of energy and momentum transfer.

The JEFF-3.1/3.1.1 libraries store all data in the internationally-accepted ENDF-6 /55/ format. Compared with JEF-2.2, a better agreement between JEFF-3.1/3.1.1-based calculations and measurements is expected in neutron transmission applications containing the following materials: Fe, O-16, Be-9, W and Na. For more details about the expected performance relative to JEF-2.2, concerning the LWR thermal reactor applications and the fast reactor applications, it is recommended to consult the official OECD-NEA Data Bank JEFF Reports 21 and 22 previously cited. Initial testing of the JEFF-3.1 file indicated that further improvements were needed in particular for Np-237 capture (updated in JEFF-3.1.1), Pu-239 fission and capture (updated in JEFF-3.1.1), Pu-242 capture, Am-241 capture, Fe-56 inelastic scattering (corrected in JEFF-3.1.1), fission product cross sections (capture cross section updated in JEFF-3.1.1 for Zr-93, Tc-99, Ru-103, Cs-135, Pm-147, Pm-148g and Eu-154), decay data and yields of short-lived fission products.

1.3 - Cross Section Processing and Testing

The calculation approach used to produce the VITJEFF311.BOLIB fine-group library is consistent, in particular, with the recommendations contained in the ANS standard “Neutron

and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations for Nuclear Power Plants” (ANSI/ANS-6.1.2-1999 (R2009) /56/). The previously cited ANS document recommends the use of VITAMIN-B6 /4/ as a reference library of group-averaged data for radiation protection and shielding calculations dedicated to light water reactor plants. Following, in general, the same data processing methodology based on NJOY and SCAMPI, the VITJEFF311.BOLIB library adopts, in particular, the same neutron and photon fine-group structures and weighting spectra used to generate VITAMIN-B6.

The data processing methodology followed in ENEA-Bologna employs both the following modular nuclear data processing systems LANL NJOY-99.259 /10/ and the ENEA-Bologna 2007 Revision /11/ of the ORNL SCAMPI /12/. Several modules of NJOY were used to process the neutron interaction, the photon production and the photon interaction data from the JEFF-3.1.1 formats to a group-averaged format.

In order to process correctly modern evaluated nuclear data like the JEFF-3.1.1 data files, it was necessary to develop an updated and corrected version of the SCAMPI system, originally developed at ORNL from the AMPX-77 /57/ system and already employed at ORNL to generate the VITAMIN-B6 data in the AMPX format. In particular, the previously cited ENEA-Bologna 2007 Revision of SCAMPI was developed, able to generate and to read data in AMPX format, and was released to OECD-NEA Data Bank and ORNL-RSICC.

In particular the ENEA-Bologna 2007 Revision of SCAMPI, through the revised and corrected SMILER module, was employed to read the double-precision GENDF binary files from the NJOY-99.259 nuclear data processing system, to translate the intermediate NJOY file into the AMPX master format for the VITJEFF311.BOLIB fine-group library and, finally, to calculate the total (prompt + delayed) neutron fission spectra and average numbers of neutrons emitted per fission, taking into account that their delayed neutron components could not be previously obtained with the original ORNL SMILER version of the SCAMPI system.

A detailed description of the data processing performed for the generation of the VITJEFF311.BOLIB fine-group library is given in Chapter 2 while the results of a validation of the library on many thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments is presented in Chapter 3.

2 - LIBRARY SPECIFICATIONS

The VITJEFF311.BOLIB library is a fine-group pseudo-problem-independent cross section library, based on the Bondarenko /9/ (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects. This library, generated in ENEA-Bologna by the Nuclear Data Group, is a coupled neutron/photon library in AMPX format for nuclear fission applications, based on the OECD-NEA Data Bank JEFF-3.1.1 /1/ /3/ evaluated nuclear data library. It has the same neutron and photon energy group structures (199 neutron groups + 42 photon groups) and general basic features as the ORNL DLC-184/VITAMIN-B6 /4/ American library in AMPX format, based on the ENDF/B-VI Release 3 /5/ US evaluated nuclear data library.

The VITJEFF311.BOLIB library was generated through an updated automatic calculation procedure based on the LANL NJOY-99.259 /10/ nuclear data processing system, with the updating “upnea049”, and the ENEA-Bologna 2007 Revision /11/ of the ORNL SCAMPI /12/

nuclear data processing system. VITJEFF311.BOLIB was extensively tested on many thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments.

A revised version of the SMILER module of the ENEA-Bologna 2007 Revision of the SCAMPI system was used to translate the fine-group data from the GENDF format into the AMPX master library format of the VITJEFF311.BOLIB library. In parallel, automatic multiplication of the term of ℓ -th order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrix by the $(2\ell + 1)$ factor was performed by the SMILER module for all the processed data files of the nuclides contained in the library.


The cross section files of VITJEFF311.BOLIB in AMPX format can be exclusively treated by the updated ENEA-Bologna 2007 Revision of the SCAMPI system which assures a high level of flexibility in the production of working cross section libraries and an evident consistency with the VITAMIN-B6 library generation methods. It is underlined, in particular, that the ENEA-Bologna revised version of the SMILER module, contained in the ENEA-Bologna 2007 Revision of the SCAMPI data processing system, permits to obtain separately the prompt neutron fission spectrum (MF=6 and MT=18), the delayed neutron fission spectrum (MF=5 and MT=455) and the total neutron fission spectrum needed, e.g., in the fixed source transport calculations for reactor radiation shielding applications. On the contrary, from the original ORNL SMILER version (see /12/), used to generate VITAMIN-B6 and VITJEF22.BOLIB /6/, it is possible to obtain only the prompt neutron component of the fission spectrum.

At present, the availability of the VITJEFF311.BOLIB library permits to obtain derived working libraries of collapsed and self-shielded cross sections, through the ENEA-Bologna 2007 Revision of the SCAMPI system. More specifically, the cross sections can be collapsed by the MALOCS module, can be self-shielded by the BONAMI module and finally can be generated in the AMPX or FIDO-ANISN /14/ format. The cross sections in AMPX format can be used by the XSDRNPM one-dimensional (1D) discrete ordinates transport code, included in the ORNL AMPX-77 /57/ and SCAMPI nuclear data processing systems, or in the ORNL SCALE-6 /58/ nuclear safety system. Concerning the cross sections in FIDO-ANISN format, they can be used by the discrete ordinates (S_N) deterministic codes ANISN-ORNL (1D), DORT (2D) and TORT (3D) of the DOORS /16/ system, by the PARTISN /30/ (1D, 2D and 3D) parallel time-dependent discrete ordinates system and, finally, by the MORSE /33/ 3D Monte Carlo stochastic code.

2.1 - Name

The present fine-group pseudo-problem-independent library, from which the BUGJEFF311.BOLIB /13/ broad-group working library was generated, is designated as VITJEFF311.BOLIB.

“VIT” suggests that the main features of the library are similar to those of the ORNL VITAMIN-B6 /4/ library and to the ENEA fine-group libraries /6/ /7/ in AMPX format with the same neutron and photon energy group structures. The “JEFF311” designation conveniently reflects the origin of the evaluated data: the JEFF-3.1.1 evaluated nuclear data library /1/ /3/. Finally, “BOLIB” means BOlogna LIBRARY and so it is indicative of the place of production of the library.

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	12	75

2.2 - Materials, Temperatures and Background Cross Sections

A set of 182 cross section files, derived from the JEFF-3.1.1 /1/ /3/ evaluated nuclear data library, was processed for the VITJEFF311.BOLIB fine-group library. In particular the complete list of the included nuclides is reported in TAB. 2.1 together with the corresponding Z atomic numbers, the JEFF-3.1.1 MAT numbers, the AMPX identifiers and a flag (YES/NO) indicating the presence of gamma-ray production data in the specific evaluated nuclear data file. It is underlined that, in this set of processed data files, only three data files correspond to natural evaluated elements (C-nat, V-nat and Ga-nat) whereas the other ones correspond to single isotope evaluated data files.

The VITJEFF311.BOLIB library contains the following set of twelve nuclides whose evaluated files were updated or corrected in the JEFF-3.1.1 evaluated data library with respect to the corresponding files contained in the JEFF-3.1 evaluated data library: the O-16, Zr-91, Zr-96, Eu-154, Np-237 and Pu-239 data files were updated while the Cl-35 Ca-46, Cr-52, Fe-56, Mo-95 and U-233 data files were corrected (see also 1.2).


Concerning, in particular, the JEFF-3.1.1 Pu-239 nuclear data file (see /1/), increased radiative capture (n,γ) MT=102 and decreased fission (n,f) MT=18 cross section values below 0.0253 eV, in the sub-thermal neutron energy region, were introduced together with revised energy dependence of ν_p (mean number of prompt neutrons per fission) MT=456 data up to 20 eV, with respect to the corresponding JEFF-3.1 Pu-239 nuclear data file.

The revised JEFF-3.1.1 Pu-239 evaluated data file is expected to correct, in particular, the reported /1/ k-effective (k_{eff}) overestimation in criticality calculations for MOX fuel and Pu solutions in thermal neutron spectrum (see also 1.2 and 3.1).

The Bondarenko /9/ (f-factor) method was used for handling neutron resonance self-shielding and temperature effects. As for VITAMIN-B6 /4/, all the 176 standard (not bound) nuclides were processed at the 4 temperatures of 300 °K, 600 °K, 1000 °K and 2100 °K and most materials were processed with 6 to 8 values for the background cross section σ_0 . These parameters are indicated in detail in TAB. 2.2, where it is possible to verify that nearly all materials were processed with the following values of σ_0 : 1, 10, 1.0E+2, 1.0E+3, 1.0E+4 and 1.0E+10 barns.

With respect to the σ_0 values used in the generation of the Fe-56 processed files in the VITAMIN-B6 (AMPX format), VITJEF22.BOLIB /6/ (AMPX format) and MATJEF22.BOLIB /26/ (MATXS format) older libraries, an additional σ_0 numerical value equal to 0.01 barns was used in the production of the Fe-56 processed file included in VITJEFF311.BOLIB as it was done for the VITJEFF31.BOLIB /7/ (AMPX format) and the MATJEFF31.BOLIB /27/ (MATXS format) libraries. This additional σ_0 numerical value improves further, through a more precise self-shielding factor interpolation, the neutron self-shielding of the Fe-56 cross sections in natural iron. Moreover the possibility of a more accurate self-shielding calculation for Fe-56 was considered useful also in LWR radiation damage analyses in the carbon steel of the pressure vessel and in the stainless steel of the reactor internals (see /4/ and /13/).

For consistency with most other similar libraries, it was decided to use infinitely dilute background cross sections ($\sigma_0 = 1.0E+10$ barns) for nuclides with the atomic number Z less

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	UTFISSM-P9H6-003	1	L	13	75

than 7, with the exception of B-11. Hence, only a background cross section with a numerical value of $1.0E+10$ barns was used for each of these nuclides.

NJOY input samples for generating the neutron and photon GENDF files for a standard nuclide are reported in APPENDIX A, respectively in TAB. A.1 and TAB. A.2 while a SMILER input sample for converting a standard nuclide file from the GENDF format to the AMPX master format is shown in TAB. A.3.

Thermal scattering cross sections were produced for six additional bound nuclides which were processed at all the temperatures (see TAB. 2.3) available in the JEFF-3.1.1 thermal scattering law data file (see /1/ and /2/): H-1 in light water, H-1 in polyethylene, H-1 in zirconium hydride (not contained in the VITAMIN-B6, VITJEF22.BOLIB and MATJEF22.BOLIB libraries), H-2 in heavy water, C in graphite and Be in beryllium metal.

Since NJOY-99.259 can manage no more than ten temperatures in one run and the JEFF-3.1.1 thermal data of H-1 in light water and C in graphite are given at eleven temperatures (see TAB. 2.3), a special patch was prepared in ENEA-Bologna in order to extend the maximum number of input values of some important parameters (such as temperature, background cross-section and so on) which is possible to insert in a single NJOY data processing run.

NJOY input samples for generating the neutron and photon GENDF files for a bound nuclide are reported in APPENDIX B, respectively in TAB. B.1 and TAB. B.2 while a SMILER input sample for converting a bound nuclide file from the GENDF format to the AMPX master format is shown in TAB. B.3.

Finally it is important to note that in total reactor power and heating calculations, the corresponding results can be heavily affected by the lack of gamma-ray production data in some JEFF-3.1.1 evaluated data files. Concerning this, it is recommended to verify carefully if the JEFF-3.1.1 data files of the nuclides involved in the calculations include gamma-ray production data (see TAB. 2.1).

TAB. 2.1

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma-Ray Production
1	H-H ₂ O	125/1	1001	YES
	H-CH ₂	125/37	1901	YES
	H-ZrH	125/7	1401	YES
	D-D ₂ O	128/11	1002	YES
	H-3	131	1003	NO
2	He-3	225	2003	NO
	He-4	228	2004	NO
3	Li-6	325	3006	YES
	Li-7	328	3007	YES
4	Be-9	425	4009	YES
	Be-9 (Thermal)	425/26	4309	YES
5	B-10	525	5010	YES
	B-11	528	5011	YES
6	C-nat	600	6012	YES
	C-nat (Graphite)	600/31	6312	YES
7	N-14	725	7014	YES
	N-15	728	7015	YES
8	O-16	825	8016	YES
	O-17	828	8017	NO
9	F-19	925	9019	YES
11	Na-23	1125	11023	YES
12	Mg-24	1225	12024	YES
	Mg-25	1228	12025	YES
	Mg-26	1231	12026	YES
13	Al-27	1325	13027	YES
14	Si-28	1425	14028	YES
	Si-29	1428	14029	YES
	Si-30	1431	14030	YES
15	P-31	1525	15031	YES
16	S-32	1625	16032	YES
	S-33	1628	16033	YES
	S-34	1631	16034	YES
	S-36	1637	16036	YES
17	Cl-35	1725	17035	YES
	Cl-37	1731	17037	YES
19	K-39	1925	19039	YES
	K-40	1928	19040	YES
	K-41	1931	19041	YES
20	Ca-40	2025	20040	YES
	Ca-42	2031	20042	YES
	Ca-43	2034	20043	YES
	Ca-44	2037	20044	YES
	Ca-46	2043	20046	YES
	Ca-48	2049	20048	YES
22	Ti-46	2225	22046	YES
	Ti-47	2228	22047	YES
	Ti-48	2231	22048	YES
	Ti-49	2234	22049	YES
	Ti-50	2237	22050	YES

TAB. 2.1 Continued

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma-Ray Production
23	V-nat	2300	23000	YES
24	Cr-50	2425	24050	YES
	Cr-52	2431	24052	YES
	Cr-53	2434	24053	YES
	Cr-54	2437	24054	YES
25	Mn-55	2525	25055	YES
26	Fe-54	2625	26054	YES
	Fe-56	2631	26056	YES
	Fe-57	2634	26057	YES
	Fe-58	2637	26058	YES
27	Co-59	2725	27059	YES
28	Ni-58	2825	28058	YES
	Ni-60	2831	28060	YES
	Ni-61	2834	28061	YES
	Ni-62	2837	28062	YES
	Ni-64	2843	28064	YES
29	Cu-63	2925	29063	YES
	Cu-65	2931	29065	YES
31	Ga-nat	3100	31000	YES
39	Y-89	3925	39089	YES
40	Zr-90	4025	40090	YES
	Zr-91	4028	40091	YES
	Zr-92	4031	40092	YES
	Zr-94	4037	40094	YES
	Zr-96	4043	40096	YES
41	Nb-93	4125	41093	YES
42	Mo-92	4225	42092	YES
	Mo-94	4231	42094	YES
	Mo-95	4234	42095	YES
	Mo-96	4237	42096	YES
	Mo-97	4240	42097	YES
	Mo-98	4243	42098	YES
	Mo-100	4249	42100	YES
47	Ag-107	4725	47107	NO
	Ag-109	4731	47109	NO
48	Cd-106	4825	48106	NO
	Cd-108	4831	48108	NO
	Cd-110	4837	48110	NO
	Cd-111	4840	48111	NO
	Cd-112	4843	48112	NO
	Cd-113	4846	48113	NO
	Cd-114	4849	48114	NO
	Cd-115m	4853	48115	NO
	Cd-116	4855	48116	NO
49	In-113	4925	49113	NO
	In-115	4931	49115	NO
50	Sn-112	5025	50112	NO
	Sn-114	5031	50114	NO
	Sn-115	5034	50115	NO

TAB. 2.1 Continued

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma-Ray Production
	Sn-116	5037	50116	NO
	Sn-117	5040	50117	NO
	Sn-118	5043	50118	NO
	Sn-119	5046	50119	NO
	Sn-120	5049	50120	NO
	Sn-122	5055	50122	NO
	Sn-123	5058	50123	NO
	Sn-124	5061	50124	NO
	Sn-125	5064	50125	NO
	Sn-126	5067	50126	NO
56	Ba-138	5649	56138	NO
63	Eu-151	6325	63151	YES
	Eu-152	6328	63152	NO
	Eu-153	6331	63153	NO
	Eu-154	6334	63154	NO
	Eu-155	6337	63155	NO
64	Gd-152	6425	64152	NO
	Gd-154	6431	64154	NO
	Gd-155	6434	64155	NO
	Gd-156	6437	64156	NO
	Gd-157	6440	64157	NO
	Gd-158	6443	64158	NO
	Gd-160	6449	64160	NO
68	Er-162	6825	68162	YES
	Er-164	6831	68164	YES
	Er-166	6837	68166	YES
	Er-167	6840	68167	YES
	Er-168	6843	68168	YES
	Er-170	6849	68170	YES
72	Hf-174	7225	72174	YES
	Hf-176	7231	72176	YES
	Hf-177	7234	72177	YES
	Hf-178	7237	72178	YES
	Hf-179	7240	72179	YES
	Hf-180	7243	72180	YES
73	Ta-181	7328	73181	YES
	Ta-182	7331	73182	NO
74	W-182	7431	74182	YES
	W-183	7434	74183	YES
	W-184	7437	74184	YES
	W-186	7443	74186	YES
75	Re-185	7525	75185	NO
	Re-187	7531	75187	NO
79	Au-197	7925	79197	YES
82	Pb-204	8225	82204	YES
	Pb-206	8231	82206	YES
	Pb-207	8234	82207	YES
	Pb-208	8237	82208	YES
83	Bi-209	8325	83209	YES

TAB. 2.1 Continued

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma-Ray Production
90	Th-230	9034	90230	NO
	Th-232	9040	90232	YES
91	Pa-231	9131	91231	NO
	Pa-233	9137	91233	NO
92	U-232	9219	92232	NO
	U-233	9222	92233	YES
	U-234	9225	92234	NO
	U-235	9228	92235	YES
	U-236	9231	92236	YES
	U-237	9234	92237	YES
	U-238	9237	92238	YES
	93	Np-237	9346	93237
Np-238		9349	93238	NO
Np-239		9352	93239	NO
94	Pu-236	9428	94236	NO
	Pu-237	9431	94237	NO
	Pu-238	9434	94238	NO
	Pu-239	9437	94239	NO
	Pu-240	9440	94240	YES
	Pu-241	9443	94241	NO
	Pu-242	9446	94242	YES
	Pu-243	9449	94243	YES
95	Pu-244	9452	94244	NO
	Am-241	9543	95241	NO
	Am-242	9546	95242	NO
	Am-242m	9547	95601	NO
96	Am-243	9549	95243	NO
	Cm-241	9628	96241	NO
	Cm-242	9631	96242	YES
	Cm-243	9634	96243	YES
	Cm-244	9637	96244	YES
	Cm-245	9640	96245	NO
	Cm-246	9643	96246	YES
	Cm-247	9646	96247	YES
Cm-248	9649	96248	YES	

TAB. 2.2

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
in the VITJEFF311.BOLIB Library.

All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]										Legendre Order	
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.		0.01
H-1	1.E+10											7
H-2	1.E+10											7
H-3	1.E+10											7
He-3	1.E+10											7
He-4	1.E+10											7
Li-6	1.E+10											7
Li-7	1.E+10											7
Be-9	1.E+10											7
B-10	1.E+10											7
B-11	1.E+10				1000.		100.		10.	1.		7
C-nat	1.E+10											7
N-14	1.E+10				1000.		100.		10.	1.		7
N-15	1.E+10				1000.		100.		10.	1.		7
O-16	1.E+10				1000.		100.		10.	1.		7
O-17	1.E+10				1000.		100.		10.	1.		7
F-19	1.E+10				1000.		100.		10.	1.		7
Na-23	1.E+10				1000.	300.	100.	50.	10.	1.		7
Mg-24	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Mg-25	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Mg-26	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Al-27	1.E+10			1.E+4	1000.		100.	50.	10.	1.		7
Si-28	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Si-29	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Si-30	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
P-31	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-32	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-33	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-34	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-36	1.E+10			1.E+4	1000.		100.		10.	1.		7
Cl-35	1.E+10			1.E+4	1000.		100.		10.	1.		7
Cl-37	1.E+10			1.E+4	1000.		100.		10.	1.		7
K-39	1.E+10			1.E+4	1000.		100.		10.	1.		7
K-40	1.E+10			1.E+4	1000.		100.		10.	1.		7
K-41	1.E+10			1.E+4	1000.		100.		10.	1.		7
Ca-40	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-42	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-43	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-44	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-46	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-48	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-46	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-47	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-48	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-49	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-50	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
V-nat	1.E+10			1.E+4	1000.		100.		10.	1.		7
Cr-50	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cr-52	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cr-53	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cr-54	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Mn-55	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Fe-54	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Fe-56	1.E+10		1.E+5	1.E+4	1000.		100.	50.	10.	1.	0.01	7
Fe-57	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Fe-58	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Co-59	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ni-58	1.E+10		1.E+5	1.E+4	1000.		100.	50.	10.	1.		7
Ni-60	1.E+10		1.E+5	1.E+4	1000.		100.	50.	10.	1.		7
Ni-61	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7

TAB. 2.2 Continued

 Background Cross Sections Values at which Bondarenko Factors Are Tabulated
 in the VITJEFF311.BOLIB Library.

All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]										Legendre Order	
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.		0.01
Ni-62	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ni-64	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cu-63	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cu-65	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ga-nat	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Y-89	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-90	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-91	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-92	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-94	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-96	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Nb-93	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-92	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-94	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-95	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-96	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-97	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-98	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-100	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ag-107	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ag-109	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-106	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-108	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-110	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-111	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-112	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-113	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-114	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-115m	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-116	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
In-113	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
In-115	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-112	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-114	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-115	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-116	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-117	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-118	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-119	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-120	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-122	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-123	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-124	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-125	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-126	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ba-138	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Eu-151	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Eu-152	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Eu-153	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Eu-154	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Eu-155	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Gd-152	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-154	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-155	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-156	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-157	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-158	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-160	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-162	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5

TAB. 2.2 Continued

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
in the VITJEFF311.BOLIB Library.

All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]										Legendre Order	
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.		0.01
Er-164	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-166	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-167	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-168	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-170	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-174	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-176	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-177	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Hf-178	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-179	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Hf-180	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ta-181	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Ta-182	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
W-182	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
W-183	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
W-184	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
W-186	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Re-185	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Re-187	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Au-197	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-204	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-206	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-207	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-208	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Bi-209	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Th-230	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Th-232	1.E+10			1.E+4	1000.	300.	100.	50.	10.	1.		5
Pa-231	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pa-233	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-232	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-233	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-234	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
U-235	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.	50.				5
U-236	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
U-237	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-238	1.E+10			1.E+4	1000.	300.	100.	50.	10.	1.		5
Np-237	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Np-238	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Np-239	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-236	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-237	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-238	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-239	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-240	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-241	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-242	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-243	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-244	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Am-241	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Am-242	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Am-242m	1.E+10		1.E+5	1.E+4	1000.							5
Am-243	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-241	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-242	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-243	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-244	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-245	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-246	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-247	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5

TAB. 2.2 Continued

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
 in the VITJEFF311.BOLIB Library.
 All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]										Legendre Order	
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1. 0.01		
Cm-248	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5


TAB. 2.3

Processed Thermal Scattering Data in the VITJEFF311.BOLIB Library.

Thermal scattering cross sections for the following bound nuclides were produced, through the THERMR module of NJOY, from the scattering matrices $S(\alpha, \beta)$ at various temperatures, included in the original JEFF-3.1.1 thermal scattering law data file:

H-1 in H₂O (light water)
H-1 in CH₂ (polyethylene)
H-1 in ZrH (zirconium hydride)
H-2 in D₂O (heavy water)
C (graphite)
Be (beryllium metal)

Nuclide	Temperature [°K]
H-1 in H ₂ O	293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800. 1000.
H-1 in CH ₂	293.6 350.
H-1 in ZrH	293.6 400. 500. 600. 700. 800. 1000. 1200.
H-2 in D ₂ O	293.6 323.6 373.6 423.6 473.6 523.6 573.6 643.9
C	293.6 400. 500. 600. 700. 800. 1000. 1200. 1600. 2000. 3000.
Be	293.6 400. 500. 600. 700. 800. 1000. 1200.

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	23	75

2.3 - Energy Group Structure

The VITJEFF311.BOLIB library adopts the same neutron and photon energy group structures as the VITAMIN-B6 /4/ library with 199 neutron energy groups (see TAB. 2.4) and 42 photon energy groups (see TAB. 2.5). The neutron and photon energy ranges are respectively included within 1.0E-05 eV and 1.9640E+07 eV for neutrons and within 1.0E+03 eV and 3.0E+07 eV for photons.

As reported in the VITAMIN-B6 library user's manual, this 199 neutron group structure was constructed as a compromise and improvement over the 174 neutron group structure used for the VITAMIN-E /19/ fine-group library, primarily conceived to treat fast neutron spectrum applications, and the 27 neutron group structure of the 27-neutron-group library, included in the SCALE /58/ system, suitable to treat criticality safety problems and out-of-core radiation shielding applications. The 27-neutron-group library has, in particular, a favourable neutron group discretization in the thermal neutron energy range whilst the resolution in the fast neutron energy range above 0.1 MeV results to be inadequate. Therefore the choice of the 199 group structure permits to treat not only fast neutron spectrum applications, through the proper neutron group structure at higher energies typical of VITAMIN-E, but also to treat physical systems with thermal neutron spectra, through the adequate group structure at lower energies of the 27-neutron-group library. Like the VITAMIN-B6 library, the VITJEFF311.BOLIB thermal neutron energy range, i.e. the range of the neutron energy groups which include upscatter, contains 36 groups and has 5.043 eV as the uppermost boundary. In particular, the thermal neutron group energy limits are listed in TAB. 2.6. As underlined in the VITAMIN-B6 library user's manual, by combining the best features of the VITAMIN-E with the 27-group neutron energy grids, the best options were obtained for creating a problem-independent energy grid for a variety of reactor designs, including thermal (water or graphite-moderated) and fast reactor systems. Consequently, problem-dependent cross section libraries can be easily derived from VITJEFF311.BOLIB, through the ENEA-Bologna 2007 Revision /11/ of the SCAMPI /12/ data processing system, without having to repeat the multi-group averaging directly from the JEFF-3.1.1 /1/ files.

The full VITJEFF311.BOLIB library neutron energy group structure given in TAB. 2.4 is identical to the corresponding structure of the VITAMIN-B6 library. The 199 group energy limits are based on the 175 groups in VITAMIN-J /20/ (an OECD-NEA Data Bank library based on the VITAMIN-C /18/ and VITAMIN-E structures) with an expanded number of thermal groups as discussed above. At higher energies, the boundaries are almost identical with the earlier VITAMIN libraries, which consist of a basic 100-group-mesh of equal lethargy width plus numerous additional boundaries to resolve resonance minima that are important for radiation shielding calculations.

The full VITJEFF311.BOLIB library photon energy group structure given in TAB. 2.5 is identical to the corresponding structure of the VITAMIN-B6 library. It is based on a combination of the 42 photon groups in the VITAMIN-J structure and the 18 group structure in the SCALE shielding library. The top energy group extends to 30 MeV, which allows proper representation of high energy gamma-rays from neutron capture at high energies. Although the cross section for capture at neutron energies between 20 and 30 MeV is small, such a reaction in some materials can produce gamma-rays with energies between 20 and 30 MeV, as reported in the VITAMIN-B6 library user's manual.

TAB. 2.4

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
1	1.9640E+07	2.3080E+06	-6.7498E-01	0.1250
2	1.7332E+07	4.2700E+05	-5.4997E-01	0.0249
3	1.6905E+07	4.1800E+05	-5.2502E-01	0.0250
4	1.6487E+07	8.0400E+05	-4.9999E-01	0.0500
5	1.5683E+07	7.6500E+05	-4.4999E-01	0.0500
6	1.4918E+07	3.6800E+05	-3.9998E-01	0.0250
7	1.4550E+07	3.5900E+05	-3.7501E-01	0.0250
8	1.4191E+07	3.5100E+05	-3.5002E-01	0.0250
9	1.3840E+07	3.4100E+05	-3.2498E-01	0.0249
10	1.3499E+07	6.5900E+05	-3.0003E-01	0.0501
11	1.2840E+07	3.1700E+05	-2.4998E-01	0.0250
12	1.2523E+07	3.0900E+05	-2.2498E-01	0.0250
13	1.2214E+07	5.9600E+05	-2.0000E-01	0.0500
14	1.1618E+07	5.6600E+05	-1.4997E-01	0.0499
15	1.1052E+07	5.3900E+05	-1.0003E-01	0.0500
16	1.0513E+07	5.1300E+05	-5.0027E-02	0.0500
17	1.0000E+07	4.8770E+05	0.0000E+00	0.0500
18	9.5123E+06	4.6390E+05	4.9999E-02	0.0500
19	9.0484E+06	4.4130E+05	9.9997E-02	0.0500
20	8.6071E+06	4.1980E+05	1.5000E-01	0.0500
21	8.1873E+06	3.9930E+05	2.0000E-01	0.0500
22	7.7880E+06	3.7980E+05	2.5000E-01	0.0500
23	7.4082E+06	3.6130E+05	3.0000E-01	0.0500
24	7.0469E+06	3.4370E+05	3.5000E-01	0.0500
25	6.7032E+06	1.1080E+05	4.0000E-01	0.0167
26	6.5924E+06	2.1610E+05	4.1667E-01	0.0333
27	6.3763E+06	3.1100E+05	4.5000E-01	0.0500
28	6.0653E+06	2.9580E+05	5.0000E-01	0.0500
29	5.7695E+06	2.8140E+05	5.5000E-01	0.0500
30	5.4881E+06	2.6760E+05	6.0000E-01	0.0500
31	5.2205E+06	2.5460E+05	6.4999E-01	0.0500
32	4.9659E+06	2.4220E+05	6.9999E-01	0.0500
33	4.7237E+06	2.3040E+05	7.4999E-01	0.0500
34	4.4933E+06	4.2760E+05	8.0000E-01	0.1000
35	4.0657E+06	3.8690E+05	9.0000E-01	0.1000
36	3.6788E+06	3.5010E+05	1.0000E+00	0.1000
37	3.3287E+06	1.6230E+05	1.1000E+00	0.0500
38	3.1664E+06	1.5450E+05	1.1500E+00	0.0500
39	3.0119E+06	1.4680E+05	1.2000E+00	0.0500
40	2.8651E+06	1.3980E+05	1.2500E+00	0.0500
41	2.7253E+06	1.3290E+05	1.3000E+00	0.0500
42	2.5924E+06	1.2640E+05	1.3500E+00	0.0500
43	2.4660E+06	8.0800E+04	1.4000E+00	0.0333
44	2.3852E+06	1.9900E+04	1.4333E+00	0.0084
45	2.3653E+06	1.9600E+04	1.4417E+00	0.0083
46	2.3457E+06	3.8800E+04	1.4500E+00	0.0167
47	2.3069E+06	7.5600E+04	1.4667E+00	0.0333
48	2.2313E+06	1.0880E+05	1.5000E+00	0.0500
49	2.1225E+06	1.0350E+05	1.5500E+00	0.0500

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
50	2.0190E+06	9.8500E+04	1.6000E+00	0.0500
51	1.9205E+06	9.3700E+04	1.6500E+00	0.0500
52	1.8268E+06	8.9100E+04	1.7000E+00	0.0500
53	1.7377E+06	8.4700E+04	1.7500E+00	0.0500
54	1.6530E+06	8.0600E+04	1.8000E+00	0.0500
55	1.5724E+06	7.6700E+04	1.8500E+00	0.0500
56	1.4957E+06	7.3000E+04	1.9000E+00	0.0500
57	1.4227E+06	6.9300E+04	1.9500E+00	0.0500
58	1.3534E+06	6.6000E+04	2.0000E+00	0.0500
59	1.2874E+06	6.2800E+04	2.0500E+00	0.0500
60	1.2246E+06	5.9800E+04	2.1000E+00	0.0500
61	1.1648E+06	5.6800E+04	2.1500E+00	0.0500
62	1.1080E+06	1.0540E+05	2.2000E+00	0.1000
63	1.0026E+06	4.0960E+04	2.3000E+00	0.0417
64	9.6164E+05	5.4460E+04	2.3417E+00	0.0583
65	9.0718E+05	4.4240E+04	2.4000E+00	0.0500
66	8.6294E+05	4.2090E+04	2.4500E+00	0.0500
67	8.2085E+05	4.0030E+04	2.5000E+00	0.0500
68	7.8082E+05	3.8080E+04	2.5500E+00	0.0500
69	7.4274E+05	3.6230E+04	2.6000E+00	0.0500
70	7.0651E+05	3.4450E+04	2.6500E+00	0.0500
71	6.7206E+05	3.2780E+04	2.7000E+00	0.0500
72	6.3928E+05	3.1180E+04	2.7500E+00	0.0500
73	6.0810E+05	2.9660E+04	2.8000E+00	0.0500
74	5.7844E+05	2.8210E+04	2.8500E+00	0.0500
75	5.5023E+05	2.6830E+04	2.9000E+00	0.0500
76	5.2340E+05	2.5530E+04	2.9500E+00	0.0500
77	4.9787E+05	4.7380E+04	3.0000E+00	0.1000
78	4.5049E+05	4.2870E+04	3.1000E+00	0.1000
79	4.0762E+05	1.9880E+04	3.2000E+00	0.0500
80	3.8774E+05	1.8910E+04	3.2500E+00	0.0500
81	3.6883E+05	3.5100E+04	3.3000E+00	0.1000
82	3.3373E+05	3.1760E+04	3.4000E+00	0.1000
83	3.0197E+05	3.4800E+03	3.5000E+00	0.0116
84	2.9849E+05	1.2800E+03	3.5116E+00	0.0043
85	2.9721E+05	2.6900E+03	3.5159E+00	0.0091
86	2.9452E+05	7.2700E+03	3.5250E+00	0.0250
87	2.8725E+05	1.4010E+04	3.5500E+00	0.0500
88	2.7324E+05	2.6000E+04	3.6000E+00	0.1000
89	2.4724E+05	1.2060E+04	3.7000E+00	0.0500
90	2.3518E+05	1.1470E+04	3.7500E+00	0.0500
91	2.2371E+05	1.0910E+04	3.8000E+00	0.0500
92	2.1280E+05	1.0380E+04	3.8500E+00	0.0500
93	2.0242E+05	9.8700E+03	3.9000E+00	0.0500
94	1.9255E+05	9.3900E+03	3.9500E+00	0.0500
95	1.8316E+05	8.9400E+03	4.0000E+00	0.0500
96	1.7422E+05	8.4900E+03	4.0500E+00	0.0500
97	1.6573E+05	8.0900E+03	4.1000E+00	0.0500
98	1.5764E+05	7.6800E+03	4.1500E+00	0.0500

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
99	1.4996E+05	7.3200E+03	4.2000E+00	0.0500
100	1.4264E+05	6.9500E+03	4.2500E+00	0.0500
101	1.3569E+05	6.6200E+03	4.3000E+00	0.0500
102	1.2907E+05	6.3000E+03	4.3500E+00	0.0500
103	1.2277E+05	5.9800E+03	4.4000E+00	0.0500
104	1.1679E+05	5.7000E+03	4.4500E+00	0.0500
105	1.1109E+05	1.3053E+04	4.5000E+00	0.1250
106	9.8037E+04	1.1520E+04	4.6250E+00	0.1250
107	8.6517E+04	4.0140E+03	4.7500E+00	0.0475
108	8.2503E+04	3.0040E+03	4.7975E+00	0.0371
109	7.9499E+04	7.5010E+03	4.8346E+00	0.0991
110	7.1998E+04	4.6190E+03	4.9337E+00	0.0663
111	6.7379E+04	1.0817E+04	5.0000E+00	0.1750
112	5.6562E+04	4.0870E+03	5.1750E+00	0.0750
113	5.2475E+04	6.1660E+03	5.2500E+00	0.1250
114	4.6309E+04	5.4410E+03	5.3750E+00	0.1250
115	4.0868E+04	6.5610E+03	5.5000E+00	0.1750
116	3.4307E+04	2.4790E+03	5.6750E+00	0.0750
117	3.1828E+04	3.3270E+03	5.7500E+00	0.1104
118	2.8501E+04	1.5010E+03	5.8604E+00	0.0541
119	2.7000E+04	9.4200E+02	5.9145E+00	0.0355
120	2.6058E+04	1.2700E+03	5.9500E+00	0.0500
121	2.4788E+04	6.1200E+02	6.0000E+00	0.0250
122	2.4176E+04	5.9700E+02	6.0250E+00	0.0250
123	2.3579E+04	1.7040E+03	6.0500E+00	0.0750
124	2.1875E+04	2.5700E+03	6.1250E+00	0.1250
125	1.9305E+04	4.2710E+03	6.2500E+00	0.2500
126	1.5034E+04	3.3250E+03	6.5000E+00	0.2500
127	1.1709E+04	1.1140E+03	6.7500E+00	0.1000
128	1.0595E+04	1.4762E+03	6.8500E+00	0.1500
129	9.1188E+03	2.0171E+03	7.0000E+00	0.2500
130	7.1017E+03	1.5709E+03	7.2500E+00	0.2500
131	5.5308E+03	1.2234E+03	7.5000E+00	0.2500
132	4.3074E+03	6.0000E+02	7.7500E+00	0.1500
133	3.7074E+03	3.5280E+02	7.9000E+00	0.1000
134	3.3546E+03	3.1920E+02	8.0000E+00	0.1000
135	3.0354E+03	2.8890E+02	8.1000E+00	0.1000
136	2.7465E+03	1.3390E+02	8.2000E+00	0.0500
137	2.6126E+03	1.2740E+02	8.2500E+00	0.0500
138	2.4852E+03	2.3650E+02	8.3000E+00	0.1000
139	2.2487E+03	2.1400E+02	8.4000E+00	0.1000
140	2.0347E+03	4.5010E+02	8.5000E+00	0.2500
141	1.5846E+03	3.5050E+02	8.7500E+00	0.2500
142	1.2341E+03	2.7298E+02	9.0000E+00	0.2500
143	9.6112E+02	2.1260E+02	9.2500E+00	0.2500
144	7.4852E+02	1.6557E+02	9.5000E+00	0.2500
145	5.8295E+02	1.2895E+02	9.7500E+00	0.2500
146	4.5400E+02	1.0043E+02	1.0000E+01	0.2500
147	3.5357E+02	7.8210E+01	1.0250E+01	0.2500

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
148	2.7536E+02	6.0910E+01	1.0500E+01	0.2500
149	2.1445E+02	4.7430E+01	1.0750E+01	0.2500
150	1.6702E+02	3.6950E+01	1.1000E+01	0.2500
151	1.3007E+02	2.8770E+01	1.1250E+01	0.2500
152	1.0130E+02	2.2407E+01	1.1500E+01	0.2500
153	7.8893E+01	1.7451E+01	1.1750E+01	0.2500
154	6.1442E+01	1.3591E+01	1.2000E+01	0.2500
155	4.7851E+01	1.0585E+01	1.2250E+01	0.2500
156	3.7266E+01	8.2430E+00	1.2500E+01	0.2500
157	2.9023E+01	6.4200E+00	1.2750E+01	0.2500
158	2.2603E+01	4.9990E+00	1.3000E+01	0.2500
159	1.7604E+01	3.8940E+00	1.3250E+01	0.2500
160	1.3710E+01	3.0330E+00	1.3500E+01	0.2500
161	1.0677E+01	2.3617E+00	1.3750E+01	0.2500
162	8.3153E+00	1.8393E+00	1.4000E+01	0.2500
163	6.4760E+00	1.4325E+00	1.4250E+01	0.2500
164	5.0435E+00	1.1156E+00	1.4500E+01	0.2500
165	3.9279E+00	8.6890E-01	1.4750E+01	0.2500
166	3.0590E+00	6.7660E-01	1.5000E+01	0.2500
167	2.3824E+00	5.2700E-01	1.5250E+01	0.2500
168	1.8554E+00	4.1040E-01	1.5500E+01	0.2500
169	1.4450E+00	1.4500E-01	1.5750E+01	0.1060
170	1.3000E+00	1.7470E-01	1.5856E+01	0.1440
171	1.1253E+00	4.5300E-02	1.6000E+01	0.0410
172	1.0800E+00	4.0000E-02	1.6041E+01	0.0380
173	1.0400E+00	4.0000E-02	1.6079E+01	0.0390
174	1.0000E+00	1.2357E-01	1.6118E+01	0.1320
175	8.7643E-01	7.6430E-02	1.6250E+01	0.0910
176	8.0000E-01	1.1744E-01	1.6341E+01	0.1590
177	6.8256E-01	5.7500E-02	1.6500E+01	0.0880
178	6.2506E-01	9.3480E-02	1.6588E+01	0.1620
179	5.3158E-01	3.1580E-02	1.6750E+01	0.0610
180	5.0000E-01	8.6010E-02	1.6811E+01	0.1890
181	4.1399E-01	4.7190E-02	1.7000E+01	0.1210
182	3.6680E-01	4.1800E-02	1.7121E+01	0.1210
183	3.2500E-01	5.0000E-02	1.7242E+01	0.1670
184	2.7500E-01	5.0000E-02	1.7409E+01	0.2010
185	2.2500E-01	4.1000E-02	1.7610E+01	0.2010
186	1.8400E-01	3.4000E-02	1.7811E+01	0.2040
187	1.5000E-01	2.5000E-02	1.8015E+01	0.1830
188	1.2500E-01	2.5000E-02	1.8198E+01	0.2230
189	1.0000E-01	3.0000E-02	1.8421E+01	0.3560
190	7.0000E-02	2.0000E-02	1.8777E+01	0.3370
191	5.0000E-02	1.0000E-02	1.9114E+01	0.2230
192	4.0000E-02	1.0000E-02	1.9337E+01	0.2880
193	3.0000E-02	9.0000E-03	1.9625E+01	0.3560
194	2.1000E-02	6.5000E-03	1.9981E+01	0.3710
195	1.4500E-02	4.5000E-03	2.0352E+01	0.3710
196	1.0000E-02	5.0000E-03	2.0723E+01	0.6930

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
197	5.0000E-03	3.0000E-03	2.1416E+01	0.9170
198	2.0000E-03	1.5000E-03	2.2333E+01	1.3860
199	5.0000E-04	4.9000E-04	2.3719E+01	3.9120
	Lower Energy		Lower Lethargy	
	1.0000E-05		2.7631E+01	

TAB. 2.5

Photon Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
1	3.0000E+07	1.0000E+07	-1.0986E+00	0.4055
2	2.0000E+07	6.0000E+06	-6.9315E-01	0.3567
3	1.4000E+07	2.0000E+06	-3.3647E-01	0.1542
4	1.2000E+07	2.0000E+06	-1.8232E-01	0.1823
5	1.0000E+07	2.0000E+06	0.0000E+00	0.2231
6	8.0000E+06	5.0000E+05	2.2314E-01	0.0645
7	7.5000E+06	5.0000E+05	2.8768E-01	0.0690
8	7.0000E+06	5.0000E+05	3.5667E-01	0.0741
9	6.5000E+06	5.0000E+05	4.3078E-01	0.0800
10	6.0000E+06	5.0000E+05	5.1083E-01	0.0870
11	5.5000E+06	5.0000E+05	5.9784E-01	0.0953
12	5.0000E+06	5.0000E+05	6.9315E-01	0.1054
13	4.5000E+06	5.0000E+05	7.9851E-01	0.1178
14	4.0000E+06	5.0000E+05	9.1629E-01	0.1335
15	3.5000E+06	5.0000E+05	1.0498E+00	0.1542
16	3.0000E+06	5.0000E+05	1.2040E+00	0.1823
17	2.5000E+06	5.0000E+05	1.3863E+00	0.2231
18	2.0000E+06	3.4000E+05	1.6094E+00	0.1863
19	1.6000E+06	1.6000E+05	1.7958E+00	0.1014
20	1.5000E+06	1.6000E+05	1.8971E+00	0.1128
21	1.3400E+06	1.0000E+04	2.0099E+00	0.0075
22	1.3300E+06	3.3000E+05	2.0174E+00	0.2852
23	1.0000E+06	2.0000E+05	2.3026E+00	0.2231
24	8.0000E+05	1.0000E+05	2.5257E+00	0.1335
25	7.0000E+05	1.0000E+05	2.6593E+00	0.1542
26	6.0000E+05	8.8000E+04	2.8134E+00	0.1586
27	5.1200E+05	2.0000E+03	2.9720E+00	0.0039
28	5.1000E+05	6.0000E+04	2.9759E+00	0.1252
29	4.5000E+05	5.0000E+04	3.1011E+00	0.1178
30	4.0000E+05	1.0000E+05	3.2189E+00	0.2877
31	3.0000E+05	1.0000E+05	3.5066E+00	0.4055
32	2.0000E+05	5.0000E+04	3.9120E+00	0.2877
33	1.5000E+05	5.0000E+04	4.1997E+00	0.4055
34	1.0000E+05	2.5000E+04	4.6052E+00	0.2877
35	7.5000E+04	5.0000E+03	4.8929E+00	0.0690
36	7.0000E+04	1.0000E+04	4.9618E+00	0.1542
37	6.0000E+04	1.5000E+04	5.1160E+00	0.2877
38	4.5000E+04	5.0000E+03	5.4037E+00	0.1178
39	4.0000E+04	1.0000E+04	5.5215E+00	0.2877
40	3.0000E+04	1.0000E+04	5.8091E+00	0.4055
41	2.0000E+04	1.0000E+04	6.2146E+00	0.6931
42	1.0000E+04	9.0000E+03	6.9078E+00	2.3026
	Lower Energy 1.0000E+03		Lower Lethargy 9.2103E+00	

TAB. 2.6

VITJEFF311.BOLIB Library Thermal Neutron Energy Range.

Group	Upper Energy [eV]	Lethargy Width	Group	Upper Energy [eV]	Lethargy Width
164	5.04350	0.250	182	0.36680	0.121
165	3.92790	0.250	183	0.32500	0.167
166	3.05900	0.250	184	0.27500	0.201
167	2.38240	0.250	185	0.22500	0.201
168	1.85540	0.250	186	0.18400	0.204
169	1.44500	0.106	187	0.15000	0.183
170	1.30000	0.144	188	0.12500	0.223
171	1.12530	0.041	189	0.10000	0.356
172	1.08000	0.038	190	0.07000	0.337
173	1.04000	0.039	191	0.05000	0.223
174	1.00000	0.132	192	0.04000	0.288
175	0.87643	0.091	193	0.03000	0.356
176	0.80000	0.159	194	0.02100	0.371
177	0.68256	0.088	195	0.01450	0.371
178	0.62506	0.162	196	0.01000	0.693
179	0.53158	0.061	197	0.00500	0.917
180	0.50000	0.189	198	0.00200	1.386
181	0.41399	0.121	199	0.00050	3.912
				Lower Energy	
				0.00001	

2.4 - Weighting Function

The neutron and photon weighting functions used to produce the VITJEFF311.BOLIB library cross sections are the same as those employed in the generation of the VITAMIN-B6 /4/ cross sections.

The neutron weighting function is of the form typically chosen for fission reactor shielding problems, i.e., it consists of a smoothly varying combination of a Maxwellian thermal spectrum, a fission spectrum, and a “1/E” slowing down spectrum. This corresponds to the IWT=4 option in the GROUPT module of the NJOY /10/ system. The breakpoint energies for the 3-region spectrum are similar to those used in VITAMIN-C /18/. The breakpoint energy between the Maxwellian and 1/E shapes is 0.125 eV. The fission temperature has been adjusted to better reflect the neutron spectrum in a thermal reactor ($\theta = 1.273$ MeV). The use of a large number of energy groups should make the exact functional form and energy break points less important compared to generating a broad-group library directly from JEFF data. The functional form of the weighting spectrum is given by the following:

Functional Form	Energy Limits	Groups
1. Maxwellian Thermal Spectrum ($kT = 0.025$ eV)		
$W_1(E) = C_1 E e^{-E/kT}$	1.0E-5 eV to 0.125 eV	188-199
2. “1/E” Slowing-Down Spectrum		
$W_2(E) = C_2/E$	0.125 eV to 820.8 keV	67-187
3. Fission Spectrum ($\theta = 1.273$ MeV)		
$W_3(E) = C_3 E^{1/2} e^{-E/\theta}$	820.8 keV to 20 MeV	1-66

A continuous weighting spectrum is achieved with the following constants: $C_1 = 9498.4 \text{ eV}^{-2}$, $C_2 = 1.0$ and $C_3 = 2.5625 \text{ MeV}^{-1.5}$. The neutron weighting function is shown in FIG. 2.1 and listed in TAB. 2.7 in a 199 group representation.

The photon weighting spectrum consists of a 1/E spectrum with a “roll-off” of the spectrum at lower energies to represent photoelectric absorption and a similar drop-off of the spectrum at higher energies corresponding to the Q-value for neutron capture. This corresponds to the IWT=3 input option in the GAMINR module of the NJOY system. The photon weighting function is shown in FIG. 2.2 and listed in TAB. 2.8 in a 42 group representation.

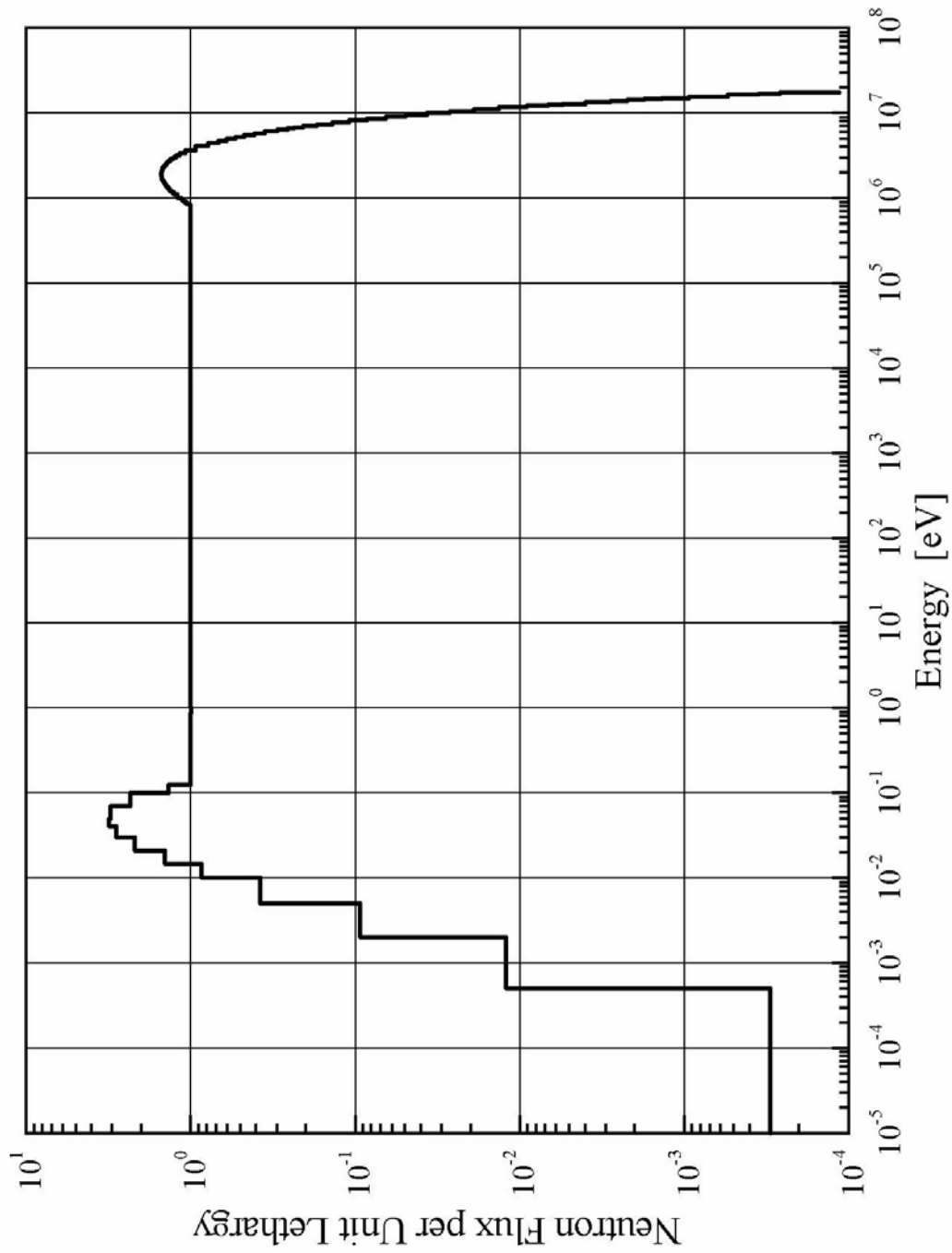


FIG. 2.1 199 Group Representation of Standard Weighting Spectrum Used to Create VITJEFF311.BOLIB Neutron Cross Sections from JEFF-3.1.1 Pointwise Data.

TAB. 2.7

Neutron Energy Weighting Spectrum for the VITJEFF311.BOLIB Library.

Group	Weight	Group	Weight	Group	Weight
1	1.423E-05	51	7.543E-02	101	5.002E-02
2	6.578E-06	52	7.516E-02	102	5.004E-02
3	8.861E-06	53	7.461E-02	103	4.994E-02
4	2.733E-05	54	7.389E-02	104	5.004E-02
5	4.690E-05	55	7.295E-02	105	1.250E-01
6	3.419E-05	56	7.181E-02	106	1.250E-01
7	4.380E-05	57	7.031E-02	107	4.751E-02
8	5.590E-05	58	6.888E-02	108	3.709E-02
9	7.036E-05	59	6.723E-02	109	9.911E-02
10	1.991E-04	60	6.552E-02	110	6.631E-02
11	1.368E-04	61	6.354E-02	111	1.750E-01
12	1.684E-04	62	1.211E-01	112	7.500E-02
13	4.576E-04	63	4.809E-02	113	1.250E-01
14	6.684E-04	64	6.474E-02	114	1.250E-01
15	9.574E-04	65	5.321E-02	115	1.750E-01
16	1.342E-03	66	5.108E-02	116	7.500E-02
17	1.843E-03	67	5.000E-02	117	1.104E-01
18	2.482E-03	68	5.000E-02	118	5.410E-02
19	3.285E-03	69	5.001E-02	119	3.551E-02
20	4.272E-03	70	4.999E-02	120	4.997E-02
21	5.465E-03	71	5.001E-02	121	2.500E-02
22	6.882E-03	72	5.000E-02	122	2.500E-02
23	8.540E-03	73	5.000E-02	123	7.501E-02
24	1.045E-02	74	5.000E-02	124	1.250E-01
25	3.951E-03	75	4.999E-02	125	2.501E-01
26	8.659E-03	76	5.001E-02	126	2.500E-01
27	1.503E-02	77	1.000E-01	127	9.998E-02
28	1.769E-02	78	1.000E-01	128	1.500E-01
29	2.058E-02	79	5.000E-02	129	2.500E-01
30	2.368E-02	80	5.000E-02	130	2.500E-01
31	2.697E-02	81	1.000E-01	131	2.500E-01
32	3.041E-02	82	1.000E-01	132	1.500E-01
33	3.397E-02	83	1.159E-02	133	1.000E-01
34	7.885E-02	84	4.297E-03	134	9.999E-02
35	9.338E-02	85	9.092E-03	135	1.000E-01
36	1.073E-01	86	2.499E-02	136	4.998E-02
37	5.848E-02	87	5.000E-02	137	4.999E-02
38	6.148E-02	88	9.999E-02	138	1.000E-01
39	6.413E-02	89	5.001E-02	139	1.000E-01
40	6.666E-02	90	5.000E-02	140	2.500E-01
41	6.879E-02	91	5.000E-02	141	2.500E-01
42	7.065E-02	92	5.001E-02	142	2.500E-01
43	4.797E-02	93	4.999E-02	143	2.500E-01
44	1.216E-02	94	5.000E-02	144	2.500E-01
45	1.212E-02	95	5.004E-02	145	2.500E-01
46	2.439E-02	96	4.996E-02	146	2.500E-01
47	4.909E-02	97	5.005E-02	147	2.500E-01
48	7.440E-02	98	4.995E-02	148	2.500E-01
49	7.503E-02	99	5.004E-02	149	2.500E-01
50	7.539E-02	100	4.995E-02	150	2.500E-01

TAB. 2.7 Continued

Neutron Energy Weighting Spectrum for the VITJEFF311.BOLIB Library.

Group	Weight	Group	Weight	Group	Weight
151	2.500E-01	168	2.500E-01	185	2.012E-01
152	2.500E-01	169	1.057E-01	186	2.043E-01
153	2.500E-01	170	1.443E-01	187	1.823E-01
154	2.500E-01	171	4.109E-02	188	3.037E-01
155	2.500E-01	172	3.774E-02	189	8.282E-01
156	2.500E-01	173	3.922E-02	190	1.038E+00
157	2.500E-01	174	1.319E-01	191	7.060E-01
158	2.500E-01	175	9.125E-02	192	8.174E-01
159	2.500E-01	176	1.588E-01	193	7.820E-01
160	2.500E-01	177	8.800E-02	194	5.360E-01
161	2.500E-01	178	1.620E-01	195	3.194E-01
162	2.500E-01	179	6.125E-02	196	2.614E-01
163	2.500E-01	180	1.888E-01	197	8.601E-02
164	2.500E-01	181	1.210E-01	198	1.684E-02
165	2.500E-01	182	1.210E-01	199	1.171E-03
166	2.500E-01	183	1.671E-01		
167	2.500E-01	184	2.007E-01		

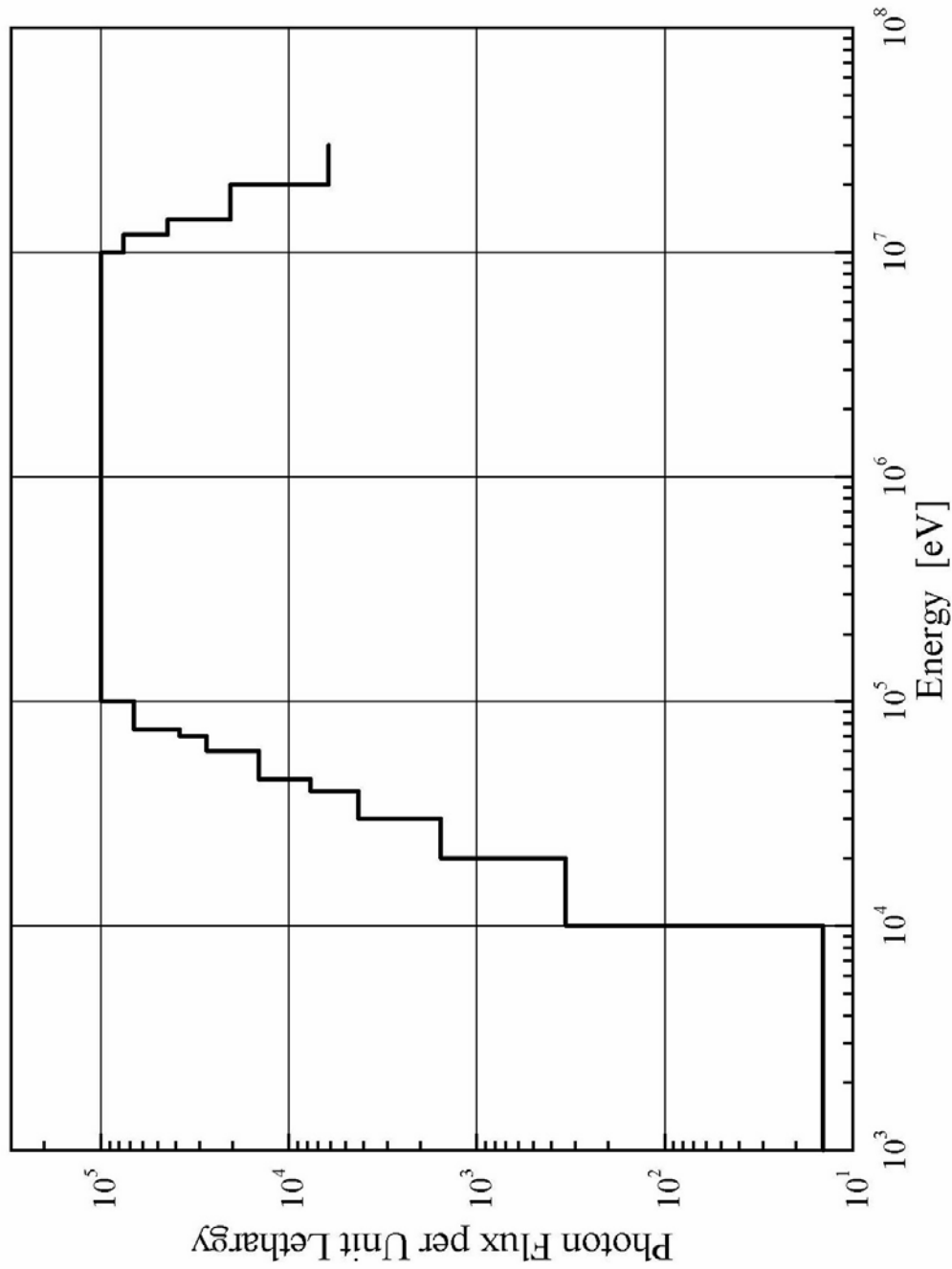



FIG. 2.2 42 Group Representation of Standard Weighting Spectrum Used to Create VITJEFF311.BOLIB Photon Cross Sections from JEFF-3.1.1 Pointwise Data.

TAB. 2.8

Photon Energy Weighting Spectrum for the VITJEFF311.BOLIB Library.

Group	Weight	Group	Weight	Group	Weight
1	2.498E+03	15	1.542E+04	29	1.178E+04
2	7.298E+03	16	1.824E+04	30	2.877E+04
3	6.824E+03	17	2.232E+04	31	4.055E+04
4	1.387E+04	18	1.864E+04	32	2.877E+04
5	2.232E+04	19	1.014E+04	33	4.055E+04
6	6.455E+03	20	1.128E+04	34	1.927E+04
7	6.901E+03	21	7.491E+02	35	2.629E+03
8	7.413E+03	22	2.852E+04	36	4.233E+03
9	8.006E+03	23	2.232E+04	37	4.163E+03
10	8.703E+03	24	1.335E+04	38	9.042E+02
11	9.534E+03	25	1.542E+04	39	1.233E+03
12	1.054E+04	26	1.586E+04	40	6.333E+02
13	1.178E+04	27	3.914E+02	41	2.333E+02
14	1.336E+04	28	1.252E+04	42	3.330E+01

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	UTFISSM-P9H6-003	1	L	37	75

2.5 - Legendre Order of Scattering

The order of scattering used for both neutrons and photons is P_7 , for nuclides with $Z=1$ through $Z=29$ (copper) and P_5 for the remainder of the nuclides. In particular, the previous values corresponding to $L=\ell$ -max, the maximum order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrix, available for each nuclide of the library, are listed in TAB. 2.2.

Most calculations are likely to be done with P_3 scattering, but for some problems, e.g., when single scatter events dominate, higher orders may be required as stated in the VITAMIN-B6 /4/ library user's manual. For the same nuclide, an identical order of scattering for both neutrons and photons was adopted in the generation of the VITAMIN-B6, VITJEFF22.BOLIB /6/, MATJEF22.BOLIB /26/, VITJEFF31.BOLIB /7/, MATJEFF31.BOLIB /27/ and VITJEFF311.BOLIB cross sections.

2.6 - Convergence Parameters

The following numerical values of the fractional error tolerances were chosen as input parameters in NJOY /10/ to generate the libraries VITJEFF311.BOLIB, VITJEFF31.BOLIB /7/ and MATJEFF31.BOLIB /27/: 0.1% for resolved resonance reconstruction and for linearization in RECONR and 0.1% for thinning in BROADR. These data have reduced numerical values with respect to the 0.2% corresponding error tolerance values used to generate VITAMIN-B6 /4/, VITJEFF22.BOLIB /6/ and MATJEF22.BOLIB /26/, chosen on the basis of the ORNL experience with the VITAMIN libraries and the experience of the NJOY users.

2.7 - Processing Codes and Procedures

The NJOY-99.259 /10/ nuclear data processing system and the ENEA-Bologna 2007 Revision /11/ of the SCAMPI /12/ nuclear data processing system were used on a Personal Computer (CPU INTEL Pentium III, 448 MB of RAM; FSF-g77 version 0.5.26 FORTRAN compiler for NJOY and f77 Absoft version 5.0 FORTRAN 77 compiler for SCAMPI) with the Linux Red Hat 7.1 operating system to generate the VITJEFF311.BOLIB library. The following modules of NJOY were used to process neutron interaction (n-n), photon production (n- γ) and photon interaction (γ - γ) data into the GENDF format, from the JEFF-3.1.1 incident neutron and photo-atomic data in ENDF-6 format. Specifically, the MODER, RECONR, BROADR, THERMR, HEATR, GASPR, PURR, GROUPE modules were used for the incident neutron data while the MODER, RECONR and GAMINR modules were used for the photo-atomic data. Then the ENEA-Bologna revised version of the SMILER module, contained in the ENEA-Bologna 2007 Revision of SCAMPI, was used to translate the fine-group data from the GENDF format into the AMPX master library format of VITJEFF311.BOLIB. The RADE module of SCAMPI was used to check and screen the data for internal consistency and "sanity", i.e. the data values are physical and within expected bounds. Then the module AIM of SCAMPI was used to convert the master cross section libraries for the standard and bound nuclide cross section files from binary to BCD format.

A brief description of the function of the NJOY and SCAMPI modules is presented in TAB. 2.9. A schematic diagram illustrating the VITJEFF311.BOLIB processing procedure to produce the standard nuclide cross section files is given in FIG. 2.3, while the procedure to produce the bound nuclide cross section files is reported in FIG. 2.4.

TAB. 2.9

Modules from the NJOY-99.259 and SCAMPI
Nuclear Data Processing Systems Used to Process VITJEFF311.BOLIB.

NJOY-99.259 System

Module	Function
MODER	Converts between ENDF standard coded mode and the NJOY blocked binary mode.
RECONR	Reconstructs point-wise cross sections from JEFF resonance parameters and interpolation schemes.
BROADR	Doppler-broadens and thins point-wise cross sections.
THERMR	Produces cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range.
HEATR	Generates heat production cross sections (KERMA factors) and damage-energy production.
GASPR	Computes gas production cross sections.
PURR	Computes probability tables and effective point-wise self-shielded cross sections in the unresolved energy range.
GROUPR	Generates self-shielded multi-group cross sections and group-to-group scattering and photon production matrices in GENDF format.
GAMINR	Computes multi-group photo-atomic cross sections, KERMA factors, group-to-group photon scattering matrices.

SCAMPI System (ENEA-Bologna 2007 Revision)

Module	Function
SMILER	Translates GENDF files produced by NJOY into AMPX master interface format.
RADE	Performs sanity and consistency tests on multi-group libraries.
AIM	Converts master cross section libraries from binary format to BCD (or vice-versa).

FIG. 2.3 Procedure for Generating the VITJEFF311.BOLIB Library in AMPX Format from JEFF-3.1.1.

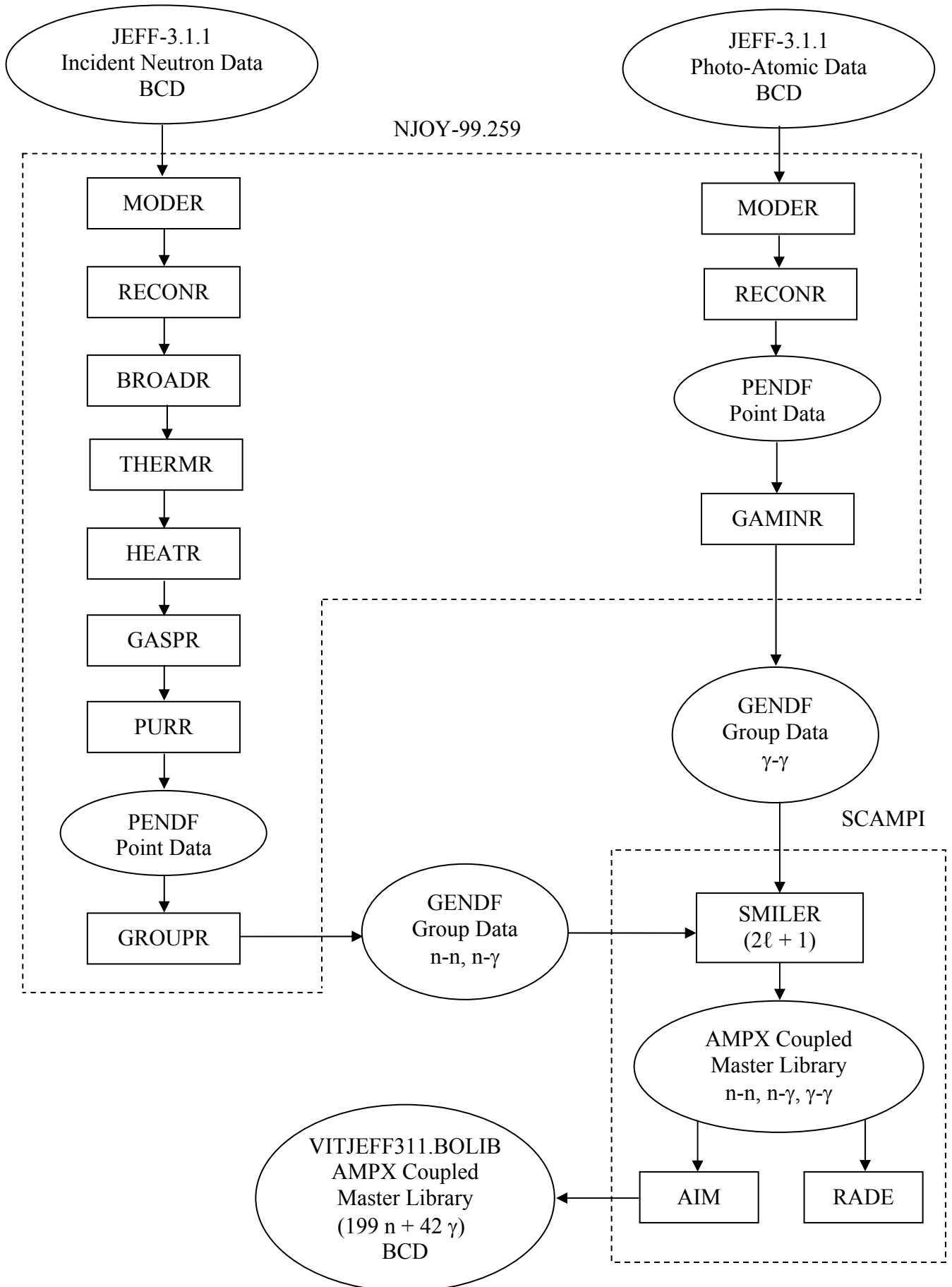
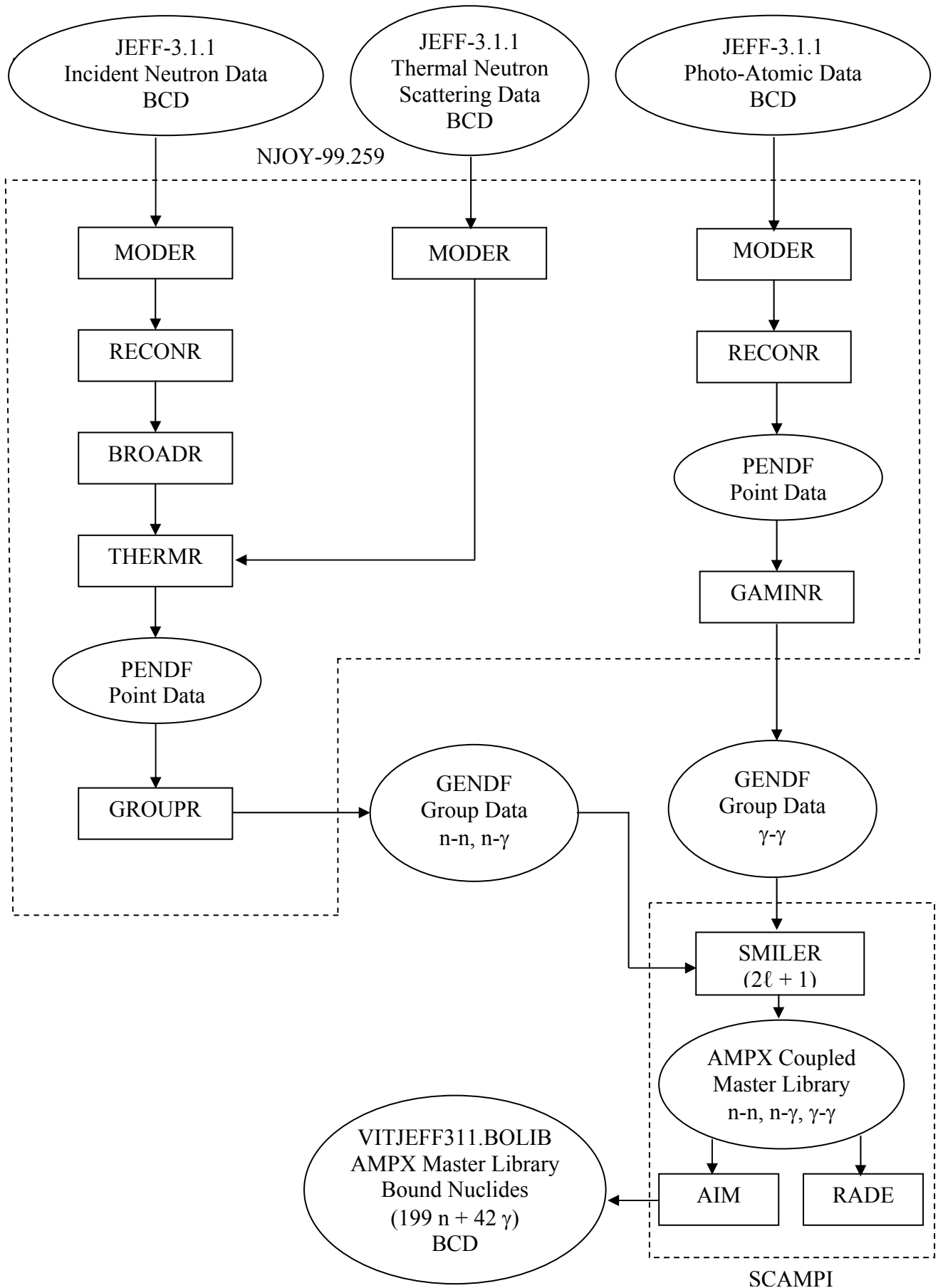



FIG. 2.4 Procedure for Generating the VITJEFF311.BOLIB Bound Nuclides in AMPX Format from JEFF-3.1.1.



 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	41	75

2.8 - Response Functions

At present only the following “response” functions are included in tabulated form in the VITJEFF311.BOLIB library package: neutron and photon group energy boundaries, neutron and photon group energy widths, neutron and photon group lethargy boundaries, neutron and photon group lethargy widths, total (prompt + delayed) neutron fission spectra (χ) for the U-235, U-238 and Pu-239 nuclides.

The total neutron fission spectra (χ) were obtained through the ENEA-Bologna 2007 Revision /11/ of the SCAMPI /12/ system which allows processing of delayed neutron spectra. In particular the BONAMI and NITAWL modules were firstly used to generate an AMPX working file for each fissile nuclide, containing infinitely dilute cross sections (background cross section $\sigma_0 = 1.0E+10$ barns) at the temperature of 300 °K. Then the fine-group χ -vectors were calculated by the ICE module with the KOPT=4 option (nuclide-dependent spectrum option) in the 1\$\$ array, i.e. using the neutron flux spectrum derived from the weighting functions corresponding to the IWT=4 option in GROUPT (see 2.4), always provided in each nuclide data file of an AMPX working library.

Then the normalization of the total neutron fission spectra (χ) to one neutron per fission was performed since the ICE module with the KOPT=4 option does not ensure a proper normalization (see /12/).

The resulting total neutron fission spectra for the U-235, U-238 and Pu-239 nuclides are reported in TAB. 2.10.

A 199 group representation of the U-235, U-238 and Pu-239 total neutron fission spectra are shown in FIG. 2.5.

TAB. 2.10

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
1	1.9640E+07	4.48634E-06	3.94788E-06	7.66615E-06
2	1.7332E+07	1.78079E-06	1.60138E-06	2.95963E-06
3	1.6905E+07	2.53131E-06	2.18954E-06	3.98909E-06
4	1.6487E+07	7.81960E-06	6.90577E-06	1.23082E-05
5	1.5683E+07	1.38064E-05	1.21619E-05	2.10980E-05
6	1.4918E+07	1.04157E-05	9.01790E-06	1.53522E-05
7	1.4550E+07	1.34932E-05	1.16883E-05	1.96454E-05
8	1.4191E+07	1.67545E-05	1.50734E-05	2.50188E-05
9	1.3840E+07	2.22685E-05	1.91597E-05	3.14141E-05
10	1.3499E+07	6.20526E-05	5.50109E-05	8.85352E-05
11	1.2840E+07	4.44331E-05	3.82734E-05	6.05660E-05
12	1.2523E+07	5.48144E-05	4.75153E-05	7.43261E-05
13	1.2214E+07	1.47663E-04	1.30673E-04	2.00851E-04
14	1.1618E+07	2.20852E-04	1.93610E-04	2.91131E-04
15	1.1052E+07	3.19940E-04	2.80900E-04	4.13668E-04
16	1.0513E+07	4.49965E-04	3.98708E-04	5.75562E-04
17	1.0000E+07	5.99347E-04	5.53062E-04	7.83175E-04
18	9.5123E+06	8.15864E-04	7.53669E-04	1.04731E-03
19	9.0484E+06	1.09025E-03	1.00782E-03	1.37538E-03
20	8.6071E+06	1.43111E-03	1.32404E-03	1.77577E-03
21	8.1873E+06	1.84619E-03	1.71003E-03	2.25512E-03
22	7.7880E+06	2.34196E-03	2.17232E-03	2.81865E-03
23	7.4082E+06	2.92300E-03	2.71586E-03	3.46956E-03
24	7.0469E+06	3.59107E-03	3.34234E-03	4.20754E-03
25	6.7032E+06	1.36032E-03	1.26761E-03	1.58118E-03
26	6.5924E+06	2.98395E-03	2.78344E-03	3.44828E-03
27	6.3763E+06	5.18124E-03	4.84220E-03	5.93333E-03
28	6.0653E+06	6.09379E-03	5.70925E-03	6.90957E-03
29	5.7695E+06	7.07732E-03	6.64938E-03	7.95391E-03
30	5.4881E+06	8.11953E-03	7.65120E-03	9.05134E-03
31	5.2205E+06	9.21733E-03	8.70945E-03	1.01952E-02
32	4.9659E+06	1.03581E-02	9.80805E-03	1.13679E-02
33	4.7237E+06	1.15305E-02	1.09448E-02	1.25648E-02
34	4.4933E+06	2.66507E-02	2.53788E-02	2.87301E-02
35	4.0657E+06	3.14387E-02	3.00347E-02	3.34139E-02
36	3.6788E+06	3.60389E-02	3.45405E-02	3.77900E-02
37	3.3287E+06	1.96127E-02	1.88410E-02	2.03681E-02
38	3.1664E+06	2.06003E-02	1.98246E-02	2.12646E-02
39	3.0119E+06	2.14575E-02	2.06917E-02	2.20251E-02
40	2.8651E+06	2.22640E-02	2.15152E-02	2.27310E-02
41	2.7253E+06	2.29178E-02	2.21992E-02	2.32859E-02
42	2.5924E+06	2.34630E-02	2.27850E-02	2.37343E-02
43	2.4660E+06	1.58803E-02	1.54561E-02	1.60097E-02
44	2.3852E+06	4.01882E-03	3.91614E-03	4.04520E-03
45	2.3653E+06	4.00035E-03	3.89954E-03	4.02398E-03
46	2.3457E+06	8.04248E-03	7.84671E-03	8.08335E-03
47	2.3069E+06	1.61455E-02	1.57754E-02	1.62007E-02
48	2.2313E+06	2.43510E-02	2.38530E-02	2.43721E-02
49	2.1225E+06	2.43972E-02	2.39736E-02	2.43506E-02

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
50	2.0190E+06	2.43373E-02	2.39899E-02	2.42303E-02
51	1.9205E+06	2.41570E-02	2.38867E-02	2.39984E-02
52	1.8268E+06	2.38688E-02	2.36694E-02	2.36653E-02
53	1.7377E+06	2.34896E-02	2.33652E-02	2.32459E-02
54	1.6530E+06	2.30563E-02	2.29963E-02	2.27777E-02
55	1.5724E+06	2.25625E-02	2.25670E-02	2.22532E-02
56	1.4957E+06	2.20254E-02	2.20962E-02	2.16849E-02
57	1.4227E+06	2.13875E-02	2.15035E-02	2.10207E-02
58	1.3534E+06	2.07795E-02	2.09350E-02	2.03925E-02
59	1.2874E+06	2.01309E-02	2.03243E-02	1.97221E-02
60	1.2246E+06	1.94995E-02	1.97386E-02	1.90615E-02
61	1.1648E+06	1.87936E-02	1.90647E-02	1.83393E-02
62	1.1080E+06	3.54692E-02	3.60894E-02	3.45371E-02
63	1.0026E+06	1.39890E-02	1.42825E-02	1.35780E-02
64	9.6164E+05	1.87407E-02	1.91761E-02	1.81573E-02
65	9.0718E+05	1.53174E-02	1.56990E-02	1.48162E-02
66	8.6294E+05	1.46587E-02	1.50698E-02	1.41464E-02
67	8.2085E+05	1.39844E-02	1.44136E-02	1.34682E-02
68	7.8082E+05	1.33529E-02	1.38066E-02	1.28256E-02
69	7.4274E+05	1.27052E-02	1.31593E-02	1.21860E-02
70	7.0651E+05	1.20692E-02	1.25259E-02	1.15595E-02
71	6.7206E+05	1.14648E-02	1.19202E-02	1.09617E-02
72	6.3928E+05	1.08856E-02	1.13527E-02	1.03819E-02
73	6.0810E+05	1.03334E-02	1.08166E-02	9.82693E-03
74	5.7844E+05	9.77173E-03	1.02396E-02	9.26605E-03
75	5.5023E+05	9.22275E-03	9.67864E-03	8.73353E-03
76	5.2340E+05	8.72070E-03	9.17890E-03	8.25128E-03
77	4.9787E+05	1.59519E-02	1.68286E-02	1.50676E-02
78	4.5049E+05	1.40749E-02	1.48626E-02	1.32738E-02
79	4.0762E+05	6.41478E-03	6.80173E-03	6.03474E-03
80	3.8774E+05	6.03571E-03	6.42696E-03	5.66134E-03
81	3.6883E+05	1.08968E-02	1.16218E-02	1.02371E-02
82	3.3373E+05	9.53176E-03	1.01784E-02	8.94473E-03
83	3.0197E+05	1.02318E-03	1.09402E-03	9.60899E-04
84	2.9849E+05	3.75444E-04	4.01535E-04	3.52413E-04
85	2.9721E+05	7.87118E-04	8.41727E-04	7.38664E-04
86	2.9452E+05	2.11554E-03	2.26292E-03	1.98357E-03
87	2.8725E+05	4.02992E-03	4.31547E-03	3.77173E-03
88	2.7324E+05	7.28865E-03	7.81679E-03	6.81516E-03
89	2.4724E+05	3.27959E-03	3.51652E-03	3.06538E-03
90	2.3518E+05	3.05510E-03	3.27803E-03	2.85379E-03
91	2.2371E+05	2.84805E-03	3.05869E-03	2.65982E-03
92	2.1280E+05	2.65307E-03	2.85222E-03	2.48060E-03
93	2.0242E+05	2.47137E-03	2.65741E-03	2.31141E-03
94	1.9255E+05	2.30820E-03	2.48433E-03	2.15161E-03
95	1.8316E+05	2.15475E-03	2.32160E-03	2.00460E-03
96	1.7422E+05	2.00338E-03	2.16015E-03	1.86326E-03
97	1.6573E+05	1.86824E-03	2.01579E-03	1.73866E-03
98	1.5764E+05	1.73602E-03	1.87426E-03	1.61744E-03

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
99	1.4996E+05	1.62100E-03	1.74717E-03	1.50793E-03
100	1.4264E+05	1.50719E-03	1.62267E-03	1.39752E-03
101	1.3569E+05	1.40544E-03	1.51266E-03	1.30014E-03
102	1.2907E+05	1.30900E-03	1.41037E-03	1.20914E-03
103	1.2277E+05	1.21423E-03	1.30842E-03	1.12171E-03
104	1.1679E+05	1.13086E-03	1.21988E-03	1.04564E-03
105	1.1109E+05	2.48766E-03	2.68860E-03	2.30789E-03
106	9.8037E+04	2.07834E-03	2.25651E-03	1.92853E-03
107	8.6517E+04	6.96572E-04	7.59306E-04	6.45577E-04
108	8.2503E+04	5.11391E-04	5.58464E-04	4.73812E-04
109	7.9499E+04	1.23807E-03	1.35848E-03	1.14576E-03
110	7.1998E+04	7.30083E-04	7.93764E-04	6.77181E-04
111	6.7379E+04	1.61274E-03	1.73743E-03	1.49681E-03
112	5.6562E+04	5.74620E-04	6.17295E-04	5.32070E-04
113	5.2475E+04	8.27758E-04	8.93520E-04	7.65796E-04
114	4.6309E+04	6.89198E-04	7.46958E-04	6.36047E-04
115	4.0868E+04	7.73059E-04	8.35209E-04	7.13264E-04
116	3.4307E+04	2.75165E-04	2.97730E-04	2.53259E-04
117	3.1828E+04	3.55949E-04	3.89019E-04	3.26245E-04
118	2.8501E+04	1.55695E-04	1.71657E-04	1.41477E-04
119	2.7000E+04	9.57272E-05	1.05607E-04	8.67927E-05
120	2.6058E+04	1.26578E-04	1.39790E-04	1.14577E-04
121	2.4788E+04	5.99585E-05	6.63017E-05	5.42148E-05
122	2.4176E+04	5.78285E-05	6.40114E-05	5.22600E-05
123	2.3579E+04	1.61386E-04	1.79092E-04	1.45764E-04
124	2.1875E+04	2.33884E-04	2.64614E-04	2.10532E-04
125	1.9305E+04	3.63276E-04	4.27517E-04	3.19686E-04
126	1.5034E+04	2.53425E-04	3.02326E-04	2.20052E-04
127	1.1709E+04	7.85115E-05	9.53192E-05	6.80818E-05
128	1.0595E+04	9.38298E-05	1.06459E-04	8.40772E-05
129	9.1188E+03	1.12985E-04	1.20666E-04	1.03061E-04
130	7.1017E+03	7.83891E-05	8.41517E-05	7.09374E-05
131	5.5308E+03	5.44406E-05	5.87428E-05	4.87847E-05
132	4.3074E+03	2.43355E-05	2.65728E-05	2.17985E-05
133	3.7074E+03	1.35173E-05	1.47549E-05	1.19892E-05
134	3.3546E+03	1.16936E-05	1.27690E-05	1.02945E-05
135	3.0354E+03	1.01218E-05	1.10814E-05	8.86445E-06
136	2.7465E+03	4.53598E-06	4.98280E-06	3.96259E-06
137	2.6126E+03	4.22137E-06	4.65081E-06	3.68442E-06
138	2.4852E+03	7.58396E-06	8.40061E-06	6.61777E-06
139	2.2487E+03	6.56777E-06	7.34044E-06	5.73968E-06
140	2.0347E+03	1.28311E-05	1.44365E-05	1.11171E-05
141	1.5846E+03	8.97493E-06	1.01691E-05	7.63463E-06
142	1.2341E+03	6.29102E-06	7.26677E-06	5.32361E-06
143	9.6112E+02	4.41967E-06	5.18909E-06	3.70017E-06
144	7.4852E+02	3.11174E-06	3.70669E-06	2.56509E-06
145	5.8295E+02	2.19649E-06	2.64935E-06	1.77240E-06
146	4.5400E+02	1.55463E-06	1.91310E-06	1.23770E-06
147	3.5357E+02	1.10342E-06	1.37540E-06	8.54833E-07

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
148	2.7536E+02	7.85624E-07	9.98676E-07	5.96637E-07
149	2.1445E+02	5.61097E-07	7.29894E-07	4.19010E-07
150	1.6702E+02	4.02281E-07	5.31605E-07	2.91008E-07
151	1.3007E+02	2.89281E-07	3.91127E-07	2.04772E-07
152	1.0130E+02	2.08874E-07	2.89126E-07	1.44637E-07
153	7.8893E+01	1.51370E-07	2.13896E-07	1.01824E-07
154	6.1442E+01	1.10117E-07	1.58499E-07	7.15353E-08
155	4.7851E+01	8.04209E-08	1.18339E-07	5.08100E-08
156	3.7266E+01	5.89565E-08	8.83326E-08	3.58919E-08
157	2.9023E+01	4.33948E-08	6.62723E-08	2.55252E-08
158	2.2603E+01	3.20561E-08	5.00089E-08	1.83412E-08
159	1.7604E+01	2.37784E-08	3.77009E-08	1.30798E-08
160	1.3710E+01	1.77013E-08	2.85686E-08	9.42107E-09
161	1.0677E+01	1.02584E-08	2.17288E-08	6.83841E-09
162	8.3153E+00	7.00407E-09	1.65386E-08	4.95594E-09
163	6.4760E+00	5.45498E-09	1.26059E-08	3.59495E-09
164	5.0435E+00	4.24822E-09	9.64013E-09	2.62909E-09
165	3.9279E+00	3.30878E-09	7.38146E-09	1.92535E-09
166	3.0590E+00	2.57650E-09	5.65931E-09	1.41392E-09
167	2.3824E+00	2.00682E-09	4.35364E-09	1.04883E-09
168	1.8554E+00	1.56281E-09	3.34837E-09	7.76228E-10
169	1.4450E+00	5.52162E-10	1.17331E-09	2.64959E-10
170	1.3000E+00	6.65259E-10	1.40701E-09	3.12785E-10
171	1.1253E+00	1.72503E-10	3.63616E-10	7.99556E-11
172	1.0800E+00	1.52320E-10	3.20643E-10	7.02072E-11
173	1.0400E+00	1.52320E-10	3.20262E-10	6.98380E-11
174	1.0000E+00	4.70556E-10	9.85567E-10	2.11945E-10
175	8.7643E-01	2.91046E-10	6.06230E-10	1.27856E-10
176	8.0000E-01	4.47213E-10	9.26529E-10	1.91640E-10
177	6.8256E-01	2.18961E-10	4.51400E-10	9.17001E-11
178	6.2506E-01	3.55973E-10	7.30810E-10	1.46093E-10
179	5.3158E-01	1.20257E-10	2.45946E-10	4.85182E-11
180	5.0000E-01	3.27527E-10	6.67844E-10	1.30001E-10
181	4.1399E-01	1.79700E-10	3.64975E-10	6.99958E-11
182	3.6680E-01	1.59175E-10	3.22478E-10	6.12136E-11
183	3.2500E-01	1.90401E-10	3.84739E-10	7.22505E-11
184	2.7500E-01	1.90401E-10	3.83650E-10	7.11922E-11
185	2.2500E-01	1.56128E-10	3.13761E-10	5.75879E-11
186	1.8400E-01	1.29472E-10	2.59617E-10	4.72161E-11
187	1.5000E-01	9.52003E-11	1.90555E-10	3.44055E-11
188	1.2500E-01	9.52003E-11	1.90286E-10	3.41410E-11
189	1.0000E-01	1.14240E-10	2.27567E-10	4.02080E-11
190	7.0000E-02	7.61602E-11	1.51013E-10	2.61360E-11
191	5.0000E-02	3.80801E-11	7.52512E-11	1.28672E-11
192	4.0000E-02	3.80801E-11	7.50970E-11	1.27334E-11
193	3.0000E-02	3.42721E-11	6.74309E-11	1.13456E-11
194	2.1000E-02	2.47521E-11	4.83001E-11	8.12658E-12
195	1.4500E-02	1.71360E-11	3.34194E-11	5.59297E-12
196	1.0000E-02	1.90401E-11	3.71324E-11	6.14635E-12

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
197	5.0000E-03	1.14240E-11	2.22794E-11	3.63687E-12
198	2.0000E-03	5.71202E-12	1.11397E-11	1.80304E-12
199	5.0000E-04	1.90400E-12	3.71321E-12	5.95697E-13
	Lower Energy			
	1.0000E-05			

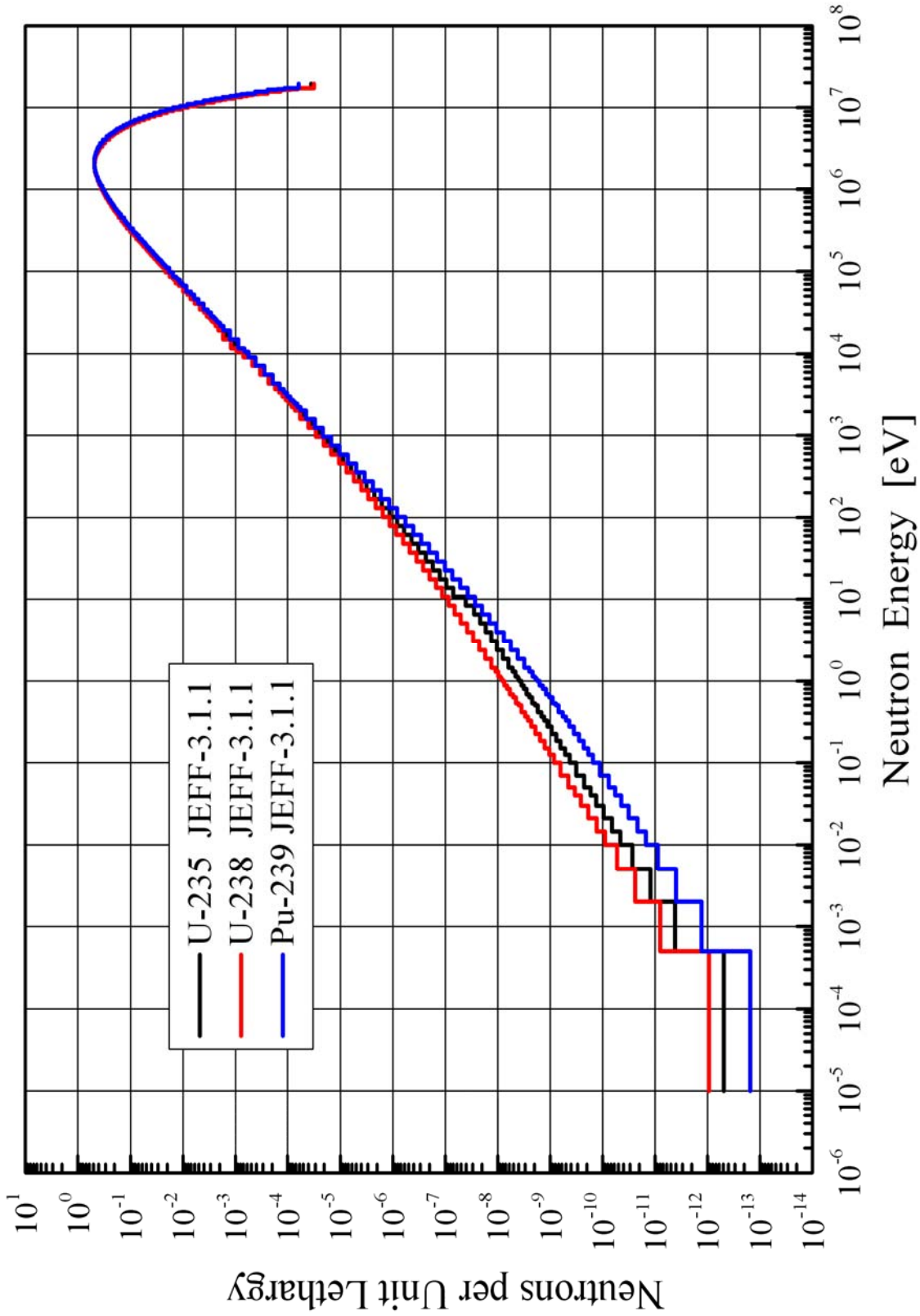



FIG. 2.5 199 Group Representation of the Total (Prompt + Delayed) Neutron Fission Spectrum for the U-235, U-238 and Pu-239 Processed Files Included in the VITJEFF311.BOLIB Library. Spectra Averaged on Incident Neutron Energies and Normalized to 1 Neutron per Fission.

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	48	75

3 - LIBRARY VALIDATION

3.1 - Reactor Physics Benchmarks

The VITJEFF311.BOLIB library was extensively tested on about 80, thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments, taking the compositional and geometrical data for the transport calculations exclusively from the ICSBEP handbook (2004 Edition) /59/ of benchmark specifications.

The k-effective (k_{eff}) results obtained with VITJEFF311.BOLIB were compared with the results previously obtained (see /7/) in ENEA-Bologna with the VITJEFF31.BOLIB /7/ library.

The ENEA-Bologna 2007 Revision /11/ of the SCAMPI /12/ system was used to prepare, through the BONAMI module, the working libraries of neutron self-shielded cross sections for the one-dimensional (1D) and two-dimensional (2D) transport calculations, respectively performed with the XSDRNPM 1D discrete ordinates transport code of the SCAMPI system and the DORT 2D discrete ordinates transport code, included in the DOORS-3.2 /16/ system.

Following the denominations reported in the ICSBEP handbook, the k-effective (k_{eff}) results obtained in the 1D and 2D transport calculations with the VITJEFF311.BOLIB library refer to HEU (Highly Enriched Uranium) benchmark experiments (TAB. 3.1), to IEU (Intermediate Enrichment Uranium) benchmark experiments (TAB. 3.2), to LEU (Low Enriched Uranium) benchmark experiments (TAB. 3.3), to a MIX (MIXed Plutonium-Uranium) benchmark experiment (TAB. 3.4), to U-233 benchmark experiments (TAB. 3.5) and to Pu-239 benchmark experiments (TAB. 3.6). The following acronyms are used in the cited tables: NU (natural uranium), DU (depleted uranium) and WC (wolfram carbide or tungsten carbide).

It is underlined that in the ICSBEP Handbook it is considered usually reasonable the assumption of a normal probability distribution for the k_{eff} values of the “experimental or benchmark-model” configurations. Consequently the k_{eff} values reported in TABs. 3.1÷3.6 are the mean values of the assumed normal distributions and their associated uncertainties correspond to one standard deviation (\pm sigma) which represents a 68% confidence level.

The k-effective (k_{eff}) results obtained with the VITJEFF311.BOLIB library are compared in the cited tables with the corresponding results obtained with the older VITJEFF31.BOLIB library. In the comparison of the k_{eff} calculated results obtained with the VITJEFF311.BOLIB library and the VITJEFF31.BOLIB older library one should take into account that, differently from VITJEFF311.BOLIB which was processed with NJOY-99.259 /10/, VITJEFF31.BOLIB was generated (see /7/) with NJOY-99.160 including a correction patch /60/ prepared in ENEA-Bologna for the GROUPE module. This action was necessary (see /7/) at the time of the data processing of VITJEFF31.BOLIB to extend the group-wise data processing capability to evaluated data files including non Cartesian interpolation schemes as, e.g., 69 JEFF-3.1 evaluated data files which could not be processed correctly through NJOY-99.160 or through all previous versions officially released. An analogous GROUPE patch, able to solve the cited problem, was officially introduced in NJOY-99 in the versions released after NJOY-99.160. The one-dimensional transport calculations in spherical geometry were performed with the XSDRNPM code, module of the SCAMPI system, in the P_5 - S_{16} approximation: P_5 corresponds to $L=\ell$ -max, the maximum order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrices and S_{16} represents the order of the flux

angular discretization. The DORT 2D discrete ordinates code, included in the DOORS-3.2 system, was exclusively employed in the simulation of the IEU-MET-FAST-007 (BIG TEN) (see TAB. 3.2) fast neutron spectrum benchmark experiment with a 2D (R,Z) cylindrical geometry calculation in the P_3 - S_8 approximation. The most relevant discrepancies of the VITJEFF311.BOLIB results, in comparison with the corresponding results obtained with the VITJEFF31.BOLIB library, are noted in the following benchmark experiments.

The VITJEFF311.BOLIB k_{eff} results, with respect to the corresponding VITJEFF31.BOLIB k_{eff} values, present an increase of about 200-300 pcm in the Low Enrichment Uranium (LEU) benchmark experiments in a thermal neutron spectrum (see TAB. 3.3). These criticality benchmark experiments are uranium solutions of uranyl nitrate, $\text{UO}_2(\text{NO}_3)$ dissolved in nitric acid (HNO_3) and diluted with distilled water (H_2O).

In the JEFF-3.1.1 O-16 re-evaluated data file, the O-16(n, α) cross section (energy threshold equal to 2.36 MeV) value below about 6.0 MeV (see /1/) was decreased with respect to the corresponding JEFF-3.1 O-16 cross section value. This modification, coupled with the high weight percentage (w%) of U-238 (effective threshold energy of the U-238 fission cross section equal to about 1.4 MeV /61/), may have probably a role to explain the cited discrepancies. On the contrary it is noted that in similar uranium solution benchmark experiments in a thermal neutron spectrum with Highly Enriched Uranium (HEU) (i.e. with low U-238 weight percentage), the k_{eff} results obtained (see TAB. 3.1) with both the cited libraries present nearly the same values.

The VITJEFF311.BOLIB library was specifically tested with particular attention on various Pu-239 criticality benchmark experiments (see TAB. 3.6).

The validation of the VITJEFF311.BOLIB library, including the processed cross sections of the JEFF-3.1.1 Pu-239 re-evaluated data file (see, in particular, 1.2 and 2.2), showed a significant correction (see TAB. 3.6) of the results of the transport calculations on the plutonium criticality experiments in a thermal neutron spectrum with respect to the corresponding results (see /7/) obtained with the VITJEFF31.BOLIB library. For example, the systematic overestimation of the k_{eff} results, observed in the analysis of the plutonium solution experiments when the JEFF-3.1 Pu-239 cross sections of the VITJEFF31.BOLIB library were employed, was corrected with a reduction of about 300-400 pcm in the VITJEFF311.BOLIB k_{eff} results, as shown in TAB. 3.6.

On the contrary the results obtained with the two libraries on the plutonium criticality experiments with fast neutron spectrum were nearly identical, as reported in TAB. 3.6. The only exception in the considered fast neutron benchmark experiments is the PU-MET-FAST-011-001 benchmark experiment (a plutonium sphere with radius equal to 4.1217 cm, reflected by 10 inches of water /59/) where the VITJEFF311.BOLIB library gave a reduced value of the k_{eff} result of about 240 pcm (see TAB. 3.6) with respect to the corresponding VITJEFF31.BOLIB k_{eff} value. This was probably due to a combined effect of the Pu-239 (in the plutonium sphere) and O-16 (in the water reflector) of the revised data in the corresponding re-evaluated files (see /1/) of the JEFF-3.1.1 nuclear data library.

3.2 - Shielding Benchmarks

At present no testing of the VITJEFF311.BOLIB library was performed on integral shielding benchmark experiments.

TAB. 3.1

VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for Highly Enriched Uranium (HEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Thermal Neutron Spectrum					
HEU-SOL-THERM-009-001	H2O	0.99900 ± (430)	1D Sph./ P5-S16	1.00189	1.00192
HEU-SOL-THERM-009-002	H2O	1.00000 ± (390)	1D Sph./ P5-S16	1.00236	1.00247
HEU-SOL-THERM-009-003	H2O	1.00000 ± (360)	1D Sph./ P5-S16	1.00166	1.00179
HEU-SOL-THERM-009-004	H2O	0.99860 ± (350)	1D Sph./ P5-S16	0.99591	0.99595
HEU-SOL-THERM-010-001	H2O	1.00000 ± (290)	1D Sph./ P5-S16	1.00123	1.00106
HEU-SOL-THERM-010-002	H2O	1.00000 ± (290)	1D Sph./ P5-S16	1.00185	1.00168
HEU-SOL-THERM-010-003	H2O	1.00000 ± (290)	1D Sph./ P5-S16	1.00044	1.00028
HEU-SOL-THERM-010-004	H2O	0.99920 ± (290)	1D Sph./ P5-S16	0.99906	0.99891
HEU-SOL-THERM-011-001	H2O	1.00000 ± (230)	1D Sph./ P5-S16	1.00523	1.00493
HEU-SOL-THERM-011-002	H2O	1.00000 ± (230)	1D Sph./ P5-S16	1.00137	1.00106
HEU-SOL-THERM-012-001	H2O	0.99990 ± (580)	1D Sph./ P5-S16	1.00111	1.00061
HEU-SOL-THERM-013-001 (ORNL-1)	--	1.00120 ± (260)	1D Sph./ P5-S16	0.99892	0.99839
HEU-SOL-THERM-013-002 (ORNL-2)	--	1.00070 ± (360)	1D Sph./ P5-S16	0.99797	0.99745
HEU-SOL-THERM-013-003 (ORNL-3)	--	1.00090 ± (360)	1D Sph./ P5-S16	0.99442	0.99391
HEU-SOL-THERM-013-004 (ORNL-4)	--	1.00030 ± (360)	1D Sph./ P5-S16	0.99599	0.99548
HEU-SOL-THERM-032 (ORNL-10)	--	1.00150 ± (260)	1D Sph./ P5-S16	0.99878	0.99812
Intermediate Neutron Spectrum					
ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{\text{inf}} \pm \Delta k_{\text{inf}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{inf}	VITJEFF31 k_{inf}
HEU-COMP-INTER-004	--	1.00000 ± (400)	Inf. Homogeneous/ P5-S16	1.00807	1.00881

TAB. 3.1 Continued

 VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
 for Highly Enriched Uranium (HEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark- Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Fast Neutron Spectrum					
HEU-MET-FAST-001-001 (GODIVA)	--	1.00000 ± (100)	1D Sph./ P5-S16	0.99533	0.99550
HEU-MET-FAST-002-001 (TOPSY)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00095	1.00112
HEU-MET-FAST-003-001	NU (2in)	1.00000 ± (500)	1D Sph./ P5-S16	0.99373	0.99392
HEU-MET-FAST-003-002	NU (3in)	1.00000 ± (500)	1D Sph./ P5-S16	0.99345	0.99363
HEU-MET-FAST-003-003	NU (4in)	1.00000 ± (500)	1D Sph./ P5-S16	0.99825	0.99843
HEU-MET-FAST-003-004	NU (5in)	1.00000 ± (300)	1D Sph./ P5-S16	0.99643	0.99661
HEU-MET-FAST-003-005	NU (7in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00071	1.00088
HEU-MET-FAST-003-006	NU (8in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00092	1.00109
HEU-MET-FAST-003-007	NU (11in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00148	1.00164
HEU-MET-FAST-003-008	WC (1.9in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00146	1.00163
HEU-MET-FAST-003-009	WC (2.9in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00364	1.00379
HEU-MET-FAST-003-010	WC (4.5in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00897	1.00911
HEU-MET-FAST-003-011	WC (6.5in)	1.00000 ± (500)	1D Sph./ P5-S16	1.01416	1.01430
HEU-MET-FAST-003-012	Ni (8in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00922	1.00943
HEU-MET-FAST-022-001	Al	1.00000 ± (190)	1D Sph./ P5-S16	0.99527	0.99543
HEU-MET-FAST-027-001	Pb	1.00000 ± (250)	1D Sph./ P5-S16	1.00052	1.00073
HEU-MET-FAST-028-001 (FLATTOP-25)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00218	1.00235
HEU-MET-FAST-057-001	Pb	1.00000 ± (200)	1D Sph./ P5-S16	0.99425	0.99449
HEU-MET-FAST-057-002	Pb	1.00000 ± (230)	1D Sph./ P5-S16	1.00122	1.00145

TAB. 3.2

VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for Intermediate Enrichment Uranium (IEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark- Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Fast Neutron Spectrum					
IEU-MET-FAST-007 (BIG TEN) Simplified Model	DU	1.00450 ± (70)	2D Cyl./ P3-S8	0.99714	0.99715
IEU-MET-FAST-007 (BIG TEN) Two Zone Model	DU	0.99480 ± (130)	2D Cyl./ P3-S8	0.99039	0.99030

TAB. 3.3

VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for Low Enriched Uranium (LEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark- Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Thermal Neutron Spectrum					
LEU-SOL-THERM-003-003	--	0.99950 ± (420)	1D Sph./ P5-S16	1.00358	1.00161
LEU-SOL-THERM-003-006	--	0.99990 ± (490)	1D Sph./ P5-S16	1.00088	0.99824
LEU-SOL-THERM-003-009	--	0.99960 ± (520)	1D Sph./ P5-S16	0.99942	0.99672

TAB. 3.4

VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for Mixed Plutonium-Uranium (MIX) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark- Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Fast Neutron Spectrum					
MIX-MET-FAST-001-001	--	1.00000 \pm (160)	1D Sph./ P5-S16	0.99740	0.99740

TAB. 3.5

VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for U-233 Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark- Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Fast Neutron Spectrum					
U233-MET-FAST-001-001 (JEZEBEL-233)	--	1.00000 \pm (100)	1D Sph./P5-S16	1.00383	1.00383
U233-MET-FAST-002-001	HEU	1.00000 \pm (100)	1D Sph./P5-S16	1.00257	1.00259
U233-MET-FAST-002-002	HEU	1.00000 \pm (110)	1D Sph./P5-S16	1.00342	1.00345
U233-MET-FAST-003-001	NU	1.00000 \pm (100)	1D Sph./P5-S16	1.00575	1.00577
U233-MET-FAST-003-002	NU	1.00000 \pm (100)	1D Sph./P5-S16	1.00719	1.00723
U233-MET-FAST-006-001 (FLATTOP-23)	NU	1.00000 \pm (140)	1D Sph./P5-S16	1.00665	1.00670

TAB. 3.6


VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for Plutonium Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Thermal Neutron Spectrum					
PU-SOL-THERM-006-001	H2O	1.00000 ± (350)	1D Sph./ P5-S16	0.99716	1.00094
PU-SOL-THERM-006-002	H2O	1.00000 ± (350)	1D Sph./ P5-S16	0.99843	1.00217
PU-SOL-THERM-006-003	H2O	1.00000 ± (350)	1D Sph./ P5-S16	0.99800	1.00164
PU-SOL-THERM-011-001	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00721	1.01069
PU-SOL-THERM-011-002	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01190	1.01536
PU-SOL-THERM-011-003	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01397	1.01735
PU-SOL-THERM-011-004	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00656	1.00990
PU-SOL-THERM-011-005 (PNL-5R)	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00364	1.00677
PU-SOL-THERM-011-006 (PNL-3R)	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99165	0.99547
PU-SOL-THERM-011-007	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99760	1.00140
PU-SOL-THERM-011-008	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99421	0.99801
PU-SOL-THERM-011-009	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99088	0.99461
PU-SOL-THERM-011-010	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00083	1.00453
PU-SOL-THERM-011-011 (PNL-4R)	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99752	1.00106
PU-SOL-THERM-011-012	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99702	1.00077
PU-SOL-THERM-021-007 (PNL-1)	--	1.00000 ± (320)	1D Sph./ P5-S16	1.00412	1.00750
PU-SOL-THERM-021-008 (PNL-2)	--	1.00000 ± (650)	1D Sph./ P5-S16	1.00226	1.00378
PU-SOL-THERM-021-009	--	1.00000 ± (320)	1D Sph./ P5-S16	1.00461	1.00788
Intermediate Neutron Spectrum					
ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{\text{eff}} \pm \Delta k_{\text{eff}}(\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJFF31 k_{eff}
PU-COMP-INTER-001	--	1.00000 ± (1100)	Inf. Homogeneous/ P5-S16	1.00110	1.00124

TAB. 3.6 Continued

VITJEFF311.BOLIB and VITJEFF31.BOLIB Criticality Calculation Results
for Plutonium Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark- Model $k_{\text{eff}} \pm \Delta k_{\text{eff}} (\text{pcm})$	Geometry/ $P_L - S_N$	VITJEFF311 k_{eff}	VITJEFF31 k_{eff}
Fast Neutron Spectrum					
PU-MET-FAST-001-001 (JEZEBEL)	--	1.00000 ± (200)	1D Sph./ P5-S16	0.99889	0.99889
PU-MET-FAST-002-001 (JEZEBEL-240)	--	1.00000 ± (200)	1D Sph./ P5-S16	1.00277	1.00277
PU-MET-FAST-006-001 (FLATTOP-PU)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00305	1.00306
PU-MET-FAST-008-001 (THOR)	Th	1.00000 ± (60)	1D Sph./ P5-S16	1.00124	1.00124
PU-MET-FAST-009-001	Al	1.00000 ± (270)	1D Sph./ P5-S16	1.00401	1.00401
PU-MET-FAST-010-001	NU	1.00000 ± (180)	1D Sph./ P5-S16	1.00091	1.00091
PU-MET-FAST-011-001	H2O	1.00000 ± (100)	1D Sph./ P5-S16	0.99943	1.00185
PU-MET-FAST-018-001	Be	1.00000 ± (300)	1D Sph./ P5-S16	1.00200	1.00202
PU-MET-FAST-023-001	Graphite	1.00000 ± (230)	1D Sph./ P5-S16	0.99850	0.99850
PU-MET-FAST-024-001	Polyethylene	1.00000 ± (200)	1D Sph./ P5-S16	0.99948	0.99949
PU-MET-FAST-030-001	Graphite	1.00000 ± (210)	1D Sph./ P5-S16	1.00395	1.00396
PU-MET-FAST-031-001	Polyethylene	1.00000 ± (210)	1D Sph./ P5-S16	1.00385	1.00391

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	56	75

4 - CONCLUSION

The ENEA-Bologna Nuclear Data Group generated the VITJEFF311.BOLIB fine-group coupled cross section library in AMPX format in the same neutron and photon energy group structures (199 n + 42 γ) of the ORNL DLC-0184/VITAMIN-B6 library. This pseudo-problem-independent library is based on the Bondarenko (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects.

The VITJEFF311.BOLIB library contains processed data derived from the OECD-NEA Data Bank JEFF-3.1.1 evaluated nuclear data library. It was produced with the NJOY-99.259 data processing system through an ENEA-Bologna automatic procedure and it was tested on several thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments.

A similar fine-group library in MATXS format, based on both the JEFF-3.1.1 and JEFF-3.1 data, was previously generated by the ENEA-Bologna Nuclear Data Group with a corrected version of NJOY-99.160 and it is in free distribution at the OECD-NEA Data Bank with the designation NEA-1847/01 ZZ MATJEFF31.BOLIB.


It is underlined that the BUGJEFF311.BOLIB broad-group working library in FIDO-ANISN format, dedicated to LWR shielding and pressure vessel dosimetry applications, was derived from VITJEFF311.BOLIB, through problem-dependent cross section collapsing and neutron self-shielding calculations performed by the ENEA-Bologna 2007 Revision of the SCAMPI nuclear data processing system. In particular, BUGJEFF311.BOLIB has the same neutron and photon group structures (47 n + 20 γ) of the ORNL DLC-0185/BUGLE-96 library, derived from VITAMIN-B6 through problem-dependent cross section collapsing. The BUGJEFF311.BOLIB library is in free distribution at the OECD-NEA Data Bank with the designation NEA-1866/01 ZZ BUGJEFF311.BOLIB.

The possibility is being studied to obtain from the VITJEFF311.BOLIB library a new broad-group working library in FIDO-ANISN format with an increased number of thermal neutron energy groups with respect to those included in the BUGLE-96 library. This to permit more accurate analyses of the thermal neutron and photon radiation damage in applications where these contributions to the total damage are not negligible.

Further testing of the VITJEFF311.BOLIB library will continue in future and it is not excluded that new response functions or additional nuclides can be added, also on the basis of possible specific requests.

An analogous data processing activity was performed also using the US ENDF/B-VII.0 nuclear data files.

It is believed, in general, that it should be very important to further promote, at the international level (UNO-IAEA, OECD-NEA, industrial organizations, R&D institutions, etc.), not only the development of fine-group general-purpose cross section libraries like VITJEFF311.BOLIB but also the generation of new working cross section libraries for radiation shielding applications, like BUGJEFF311.BOLIB, dedicated to various types of Generation III and IV nuclear fission reactors with different compositional, geometrical and

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	57	75

spectral specifications. In fact the availability of these working libraries, derived through problem-dependent cross section collapsing from the previously cited general-purpose libraries, could promote, in particular, the use of the three-dimensional deterministic codes in radiation shielding and radiation damage calculations for nuclear safety. This is increasingly requested, due to the fact that these transport codes (TORT, PARTISN, KATRIN, etc.) reached in the last years an effective capability of complex geometry description, through modern dedicated pre/post-processor systems (BOT3P, TORTWARE, etc.) for the automatic generation of the spatial meshes.

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APPENDIX A

Samples of NJOY and SMILER Input Listings for a Standard Nuclide

TAB. A.1

Sample of NJOY Input for Generating the Neutron GENDF File for a Standard Nuclide.

```

moder
1 -21 /
' JEFF-3.1.1/U_235 '/
20 9228 /
0 /
reconr
-21 -22 /
' JEFF-3.1.1/U_235 '/
9228 1 / mat ncards ngrid
0.001 / 0. 7 20*err err/10000 /err tempr ndigit errmax errint
' JEFF-3.1.1/U_235 '/
0 /
broadr
-21 -22 -23 /
9228 4 0 0 0. / mat ntemp2 istart istrap temp1
0.001 / 1.E6 0.002 0.0000001 / errthn thnmax errmax errint
300. 600. 1000. 2100.
0 / next mat (0 - terminate)
thermr
0 -23 -24 / tape_with_mf7 pendf_old pendf_new
0 9228 16 4 1 0 1 221 1 /matmf7 mat nbin ntemp iinc icoh natom mtref
300. 600. 1000. 2100.
0.01 5.0435 / tolerance emax
heatr
-21 -24 -26 /
9228 6 0 0 0 0 / matd npk nqa ntemp local iprint
302 304 318 402 442 444 /
purr
-21 -26 -27 /
9228 4 7 20 50 1 0 / mat ntem nsig nbin nladr
300. 600. 1000. 2100.
1.e10 1.e6 1.e5 1.e4 1.e3 1.e2 5.e1
0 /
gaspr
-21 -27 -28 /
groupr
-21 -28 0 -30
9228 1 1 4 5 4 7 1 / mat ign igg iwt lord ntemp nsig iprint
' JEFF-3.1.1/U_235 '/
300. 600. 1000. 2100. /tem
1.e10 1.e6 1.e5 1.e4 1.e3 1.e2 5.e1 /sig
199 / VITAMIN-B6 neutron energy groups
1.0000E-05 5.0000E-04 2.0000E-03 5.0000E-03 1.0000E-02 1.4500E-02
2.1000E-02 3.0000E-02 4.0000E-02 5.0000E-02 7.0000E-02 1.0000E-01
1.2500E-01 1.5000E-01 1.8400E-01 2.2500E-01 2.7500E-01 3.2500E-01
3.6680E-01 4.1399E-01 5.0000E-01 5.3158E-01 6.2506E-01 6.8256E-01
8.0000E-01 8.7643E-01 1.0000E+00 1.0400E+00 1.0800E+00 1.1253E+00
1.3000E+00 1.4450E+00 1.8554E+00 2.3824E+00 3.0590E+00 3.9279E+00
5.0435E+00 6.4760E+00 8.3153E+00 1.0677E+01 1.3710E+01 1.7604E+01
2.2603E+01 2.9023E+01 3.7266E+01 4.7851E+01 6.1442E+01 7.8893E+01
1.0130E+02 1.3007E+02 1.6702E+02 2.1445E+02 2.7536E+02 3.5357E+02
4.5400E+02 5.8295E+02 7.4852E+02 9.6112E+02 1.2341E+03 1.5846E+03
2.0347E+03 2.2487E+03 2.4852E+03 2.6126E+03 2.7465E+03 3.0354E+03
    
```


TAB. A.1 Continued

Sample of NJOY Input for Generating the Neutron GENDF File for a Standard Nuclide.

```

3.3546E+03 3.7074E+03 4.3074E+03 5.5308E+03 7.1017E+03 9.1188E+03
1.0595E+04 1.1709E+04 1.5034E+04 1.9305E+04 2.1875E+04 2.3579E+04
2.4176E+04 2.4788E+04 2.6058E+04 2.7000E+04 2.8501E+04 3.1828E+04
3.4307E+04 4.0868E+04 4.6309E+04 5.2475E+04 5.6562E+04 6.7379E+04
7.1998E+04 7.9499E+04 8.2503E+04 8.6517E+04 9.8037E+04 1.1109E+05
1.1679E+05 1.2277E+05 1.2907E+05 1.3569E+05 1.4264E+05 1.4996E+05
1.5764E+05 1.6573E+05 1.7422E+05 1.8316E+05 1.9255E+05 2.0242E+05
2.1280E+05 2.2371E+05 2.3518E+05 2.4724E+05 2.7324E+05 2.8725E+05
2.9452E+05 2.9721E+05 2.9849E+05 3.0197E+05 3.3373E+05 3.6883E+05
3.8774E+05 4.0762E+05 4.5049E+05 4.9787E+05 5.2340E+05 5.5023E+05
5.7844E+05 6.0810E+05 6.3928E+05 6.7206E+05 7.0651E+05 7.4274E+05
7.8082E+05 8.2085E+05 8.6294E+05 9.0718E+05 9.6164E+05 1.0026E+06
1.1080E+06 1.1648E+06 1.2246E+06 1.2874E+06 1.3534E+06 1.4227E+06
1.4957E+06 1.5724E+06 1.6530E+06 1.7377E+06 1.8268E+06 1.9205E+06
2.0190E+06 2.1225E+06 2.2313E+06 2.3069E+06 2.3457E+06 2.3653E+06
2.3852E+06 2.4660E+06 2.5924E+06 2.7253E+06 2.8651E+06 3.0119E+06
3.1664E+06 3.3287E+06 3.6788E+06 4.0657E+06 4.4933E+06 4.7237E+06
4.9659E+06 5.2205E+06 5.4881E+06 5.7695E+06 6.0653E+06 6.3763E+06
6.5924E+06 6.7032E+06 7.0469E+06 7.4082E+06 7.7880E+06 8.1873E+06
8.6071E+06 9.0484E+06 9.5123E+06 1.0000E+07 1.0513E+07 1.1052E+07
1.1618E+07 1.2214E+07 1.2523E+07 1.2840E+07 1.3499E+07 1.3840E+07
1.4191E+07 1.4550E+07 1.4918E+07 1.5683E+07 1.6487E+07 1.6905E+07
1.7332E+07 1.9640E+07 /
42 / VITAMIN-B6 photon energy groups
1.0000E+03 1.0000E+04 2.0000E+04 3.0000E+04 4.0000E+04 4.5000E+04
6.0000E+04 7.0000E+04 7.5000E+04 1.0000E+05 1.5000E+05 2.0000E+05
3.0000E+05 4.0000E+05 4.5000E+05 5.1000E+05 5.1200E+05 6.0000E+05
7.0000E+05 8.0000E+05 1.0000E+06 1.3300E+06 1.3400E+06 1.5000E+06
1.6600E+06 2.0000E+06 2.5000E+06 3.0000E+06 3.5000E+06 4.0000E+06
4.5000E+06 5.0000E+06 5.5000E+06 6.0000E+06 6.5000E+06 7.0000E+06
7.5000E+06 8.0000E+06 1.0000E+07 1.2000E+07 1.4000E+07 2.0000E+07
3.0000E+07 /
0.125 0.025 8.2085E+05 1.273E+06 /eb tb ec tc
3 / tem1
3 452 /
3 455 / nu delay
3 456 / nu prompt
5 455 / delay spectrum
3 221 /
3 251 /
3 252 /
3 253 /
3 259 /
6 /
6 221 /
16 /
0 /
3 / tem2
6 2 /
6 221 /
16 /
0 /
3 / tem3

```

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	67	75


TAB. A.1 Continued.

Sample of NJOY Input for Generating the Neutron GENDF File for a Standard Nuclide.

```

6 2 /
6 221 /
16 /
0 /
3 / tem4
6 2 /
6 221 /
16 /
0 /
0 /
stop

```

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	68	75


TAB. A.2

Sample of NJOY Input for Generating the Photon GENDF File for a Standard Nuclide.

```

moder
20 -21
reconr
-21 -22
* JEFF-3.1.1/U_nat */
9200 0 / mat ncards ngrid
0.001 / 0. 7 20*err err/10000 /err tempr ndigit errmax errint
0 /
gaminr
-21 -22 0 -30
9200 1 3 5 0 /mat igg iwt lord iprint
* JEFF-3.1.1/U_nat */
42 / VITAMIN-B6 photon energy groups
1.0000E+03 1.0000E+04 2.0000E+04 3.0000E+04 4.0000E+04 4.5000E+04
6.0000E+04 7.0000E+04 7.5000E+04 1.0000E+05 1.5000E+05 2.0000E+05
3.0000E+05 4.0000E+05 4.5000E+05 5.1000E+05 5.1200E+05 6.0000E+05
7.0000E+05 8.0000E+05 1.0000E+06 1.3300E+06 1.3400E+06 1.5000E+06
1.6600E+06 2.0000E+06 2.5000E+06 3.0000E+06 3.5000E+06 4.0000E+06
4.5000E+06 5.0000E+06 5.5000E+06 6.0000E+06 6.5000E+06 7.0000E+06
7.5000E+06 8.0000E+06 1.0000E+07 1.2000E+07 1.4000E+07 2.0000E+07
3.0000E+07 /
-1 /
0 /
stop

```

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	69	75


TAB. A.3

Sample of SMILER Input for Converting a Standard Nuclide File from the GENDF Format to the AMPX Master Format.

```

=shell
rm ft3* ft2* 2>/dev/null
ln -sf U_235 ft30f001
ln -sf U ft32f001
end
=smiler
-1$$ 1000000
0$$ 20 -30 0 -32
1$$ 92235 E
2$$ 221 1007
    0 0 E
6$$ 10000 1024
t
U_235 njoy-99.259 standard wgt j3119228vj30003090509
vitjeff311 coupled cross section library
    199 neutron groups - 42 gamma groups
    data is from jeff-3.1.1
    library created /09/05/09
end
=rade
1$$ 20 E
2$$ a2 2 0 E
t
end
=aim
0$$ 20 21
1$$ 0
2$$ 0 -1 0 0 T
end
=shell
mv ft21f001 U_235.jeff311_ampx
end

```

 Centro Ricerche Bologna	Sigla di identificazione UTFISSM-P9H6-003	Rev. 1	Distrib. L	Pag. 70	di 75
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APPENDIX B

Samples of NJOY and SMILER Input Listings for a Bound Nuclide


TAB. B.1

Sample of NJOY Input for Generating the Neutron GENDF File for a Bound Nuclide.

```

moder
1 -22 /
' JEFF-3.1.1/H_1 '/
20 125 /
0 /
moder
1 -23 /
' JEFF-3.1.1/H_H2O '/
21 1 /
0 /
reconr
-22 -24
' JEFF-3.1.1/H_1 '/
125 0/
0.001 0. 7 /
0/
broadr
-22 -24 -25
125 11 / 0 0 / mat ntemp istory
0.001 /
293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800. 1000. /tem
0/
thermr
-23 -25 -26
1 125 16 11 4 0 2 222 1
293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800. 1000. /tem
0.01 5.0435
groupr
-22 -26 0 -30 /
125 1 1 4 7 11 1 0 /mat ign igg iwt lord ntemp nsigz iprint
' JEFF-3.1.1/H_H2O '/
293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800. 1000. /tem
1.e10
199 / VITAMIN-B6 neutron energy groups
1.0000E-05 5.0000E-04 2.0000E-03 5.0000E-03 1.0000E-02 1.4500E-02
2.1000E-02 3.0000E-02 4.0000E-02 5.0000E-02 7.0000E-02 1.0000E-01
1.2500E-01 1.5000E-01 1.8400E-01 2.2500E-01 2.7500E-01 3.2500E-01
3.6680E-01 4.1399E-01 5.0000E-01 5.3158E-01 6.2506E-01 6.8256E-01
8.0000E-01 8.7643E-01 1.0000E+00 1.0400E+00 1.0800E+00 1.1253E+00
1.3000E+00 1.4450E+00 1.8554E+00 2.3824E+00 3.0590E+00 3.9279E+00
5.0435E+00 6.4760E+00 8.3153E+00 1.0677E+01 1.3710E+01 1.7604E+01
2.2603E+01 2.9023E+01 3.7266E+01 4.7851E+01 6.1442E+01 7.8893E+01
1.0130E+02 1.3007E+02 1.6702E+02 2.1445E+02 2.7536E+02 3.5357E+02
4.5400E+02 5.8295E+02 7.4852E+02 9.6112E+02 1.2341E+03 1.5846E+03
2.0347E+03 2.2487E+03 2.4852E+03 2.6126E+03 2.7465E+03 3.0354E+03
3.3546E+03 3.7074E+03 4.3074E+03 5.5308E+03 7.1017E+03 9.1188E+03
1.0595E+04 1.1709E+04 1.5034E+04 1.9305E+04 2.1875E+04 2.3579E+04
2.4176E+04 2.4788E+04 2.6058E+04 2.7000E+04 2.8501E+04 3.1828E+04
3.4307E+04 4.0868E+04 4.6309E+04 5.2475E+04 5.6562E+04 6.7379E+04
7.1998E+04 7.9499E+04 8.2503E+04 8.6517E+04 9.8037E+04 1.1109E+05
1.1679E+05 1.2277E+05 1.2907E+05 1.3569E+05 1.4264E+05 1.4996E+05
1.5764E+05 1.6573E+05 1.7422E+05 1.8316E+05 1.9255E+05 2.0242E+05
2.1280E+05 2.2371E+05 2.3518E+05 2.4724E+05 2.7324E+05 2.8725E+05

```

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	72	75

TAB. B.1 Continued

Sample of NJOY Input for Generating the Neutron GENDF File for a Bound Nuclide.

```

2.9452E+05 2.9721E+05 2.9849E+05 3.0197E+05 3.3373E+05 3.6883E+05
3.8774E+05 4.0762E+05 4.5049E+05 4.9787E+05 5.2340E+05 5.5023E+05
5.7844E+05 6.0810E+05 6.3928E+05 6.7206E+05 7.0651E+05 7.4274E+05
7.8082E+05 8.2085E+05 8.6294E+05 9.0718E+05 9.6164E+05 1.0026E+06
1.1080E+06 1.1648E+06 1.2246E+06 1.2874E+06 1.3534E+06 1.4227E+06
1.4957E+06 1.5724E+06 1.6530E+06 1.7377E+06 1.8268E+06 1.9205E+06
2.0190E+06 2.1225E+06 2.2313E+06 2.3069E+06 2.3457E+06 2.3653E+06
2.3852E+06 2.4660E+06 2.5924E+06 2.7253E+06 2.8651E+06 3.0119E+06
3.1664E+06 3.3287E+06 3.6788E+06 4.0657E+06 4.4933E+06 4.7237E+06
4.9659E+06 5.2205E+06 5.4881E+06 5.7695E+06 6.0653E+06 6.3763E+06
6.5924E+06 6.7032E+06 7.0469E+06 7.4082E+06 7.7880E+06 8.1873E+06
8.6071E+06 9.0484E+06 9.5123E+06 1.0000E+07 1.0513E+07 1.1052E+07
1.1618E+07 1.2214E+07 1.2523E+07 1.2840E+07 1.3499E+07 1.3840E+07
1.4191E+07 1.4550E+07 1.4918E+07 1.5683E+07 1.6487E+07 1.6905E+07
1.7332E+07 1.9640E+07 /
42 / VITAMIN-B6 photon energy groups
1.0000E+03 1.0000E+04 2.0000E+04 3.0000E+04 4.0000E+04 4.5000E+04
6.0000E+04 7.0000E+04 7.5000E+04 1.0000E+05 1.5000E+05 2.0000E+05
3.0000E+05 4.0000E+05 4.5000E+05 5.1000E+05 5.1200E+05 6.0000E+05
7.0000E+05 8.0000E+05 1.0000E+06 1.3300E+06 1.3400E+06 1.5000E+06
1.6600E+06 2.0000E+06 2.5000E+06 3.0000E+06 3.5000E+06 4.0000E+06
4.5000E+06 5.0000E+06 5.5000E+06 6.0000E+06 6.5000E+06 7.0000E+06
7.5000E+06 8.0000E+06 1.0000E+07 1.2000E+07 1.4000E+07 2.0000E+07
3.0000E+07 /
0.125 0.025 8.2085E+05 1.273E+06 /eb tb ec tc
3 / tem1
3 222 /
3 251 /
3 252 /
3 253 /
3 259 /
6 /
6 222 /
16 /
0 /
3 / tem2
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem3
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem4
3 222 /
6 2 /
6 222 /
16 /
0 /

```



TAB. B.1 Continued

Sample of NJOY Input for Generating the Neutron GENDF File for a Bound Nuclide.

```

3 / tem5
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem6
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem7
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem8
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem9
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem10
3 222 /
6 2 /
6 222 /
16 /
0 /
3 / tem11
3 222 /
6 2 /
6 222 /
16 /
0 /
0 /
stop

```

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	74	75


TAB. B.2

Sample of NJOY Input for Generating the Photon GENDF File for a Bound Nuclide.

```

moder
20 -21
reconr
-21 -22
* JEFF-3.1.1/H */
100 0 / mat ncards ngrid
0.001 / 0. 7 20*err err/10000 /err tempr ndigit errmax errint
0 /
gaminr
-21 -22 0 -30
100 1 3 7 0 /mat igg iwt lord iprint
* JEFF-3.1.1/H */
42 / VITAMIN-B6 photon energy groups
1.0000E+03 1.0000E+04 2.0000E+04 3.0000E+04 4.0000E+04 4.5000E+04
6.0000E+04 7.0000E+04 7.5000E+04 1.0000E+05 1.5000E+05 2.0000E+05
3.0000E+05 4.0000E+05 4.5000E+05 5.1000E+05 5.1200E+05 6.0000E+05
7.0000E+05 8.0000E+05 1.0000E+06 1.3300E+06 1.3400E+06 1.5000E+06
1.6600E+06 2.0000E+06 2.5000E+06 3.0000E+06 3.5000E+06 4.0000E+06
4.5000E+06 5.0000E+06 5.5000E+06 6.0000E+06 6.5000E+06 7.0000E+06
7.5000E+06 8.0000E+06 1.0000E+07 1.2000E+07 1.4000E+07 2.0000E+07
3.0000E+07 /
-1 /
0 /
stop

```

 Centro Ricerche Bologna	Sigla di identificazione	Rev.	Distrib.	Pag.	di
	UTFISSM-P9H6-003	1	L	75	75

TAB. B.3

Sample of SMILER Input for Converting a Bound Nuclide File from the GENDF Format to the AMPX Master Format.

```

=shell
rm ft3* ft2* 2>/dev/null
ln -sf H_H2O ft30f001
ln -sf H ft32f001
end
=smiler
-1$$ 1000000
0$$ 20 -30 0 -32
1$$ 1001 E
2$$ 222 1007
    0 0 E
6$$ 10000 1024
t
H_H2O njoy-99.259 standard wgt j3110125vj30003090509
vitjeff311 coupled cross section library
    199 neutron groups - 42 gamma groups
    data is from jeff-3.1.1
    library created /09/05/09
end
=rade
1$$ 20 E
2$$ a2 2 0 E
t
end
=aim
0$$ 20 21
1$$ 0
2$$ 0 -1 0 0 T
end
=shell
mv ft20f001 H_H2O.jeff311_ampx
end

```