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# The JEFF-3.0/A Neutron Activation File—New Features, Validation, and Usage

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**Abstract.** The reasons for the conversion of the European Activation File, EAF into ENDF-6 format are threefold. First, it significantly enhances the JEFF-3.0 release by the addition of an activation file. Second, to considerably increase its usage by using a recognized, official file format, allowing existing plug-in processes to be effective; and third, to move towards a universal nuclear data file in contrast to the current separate general and special-purpose files. The format chosen for the JEFF-3.0/A file uses reaction cross sections (MF-3), cross sections (MF-10), and multiplicities (MF-9). Having the data in ENDF-6 format allows the ENDF suite of utilities and checker codes to be used alongside many other utility, visualizing, and processing codes. It is based on the EAF activation file used for many applications from fission to fusion, including dosimetry, inventories, depletion-transmutation, and geophysics. JEFF-3.0/A takes advantage of four generations of EAF files. Extensive benchmarking activities on these files provide feedback and validation with integral measurements. These, in parallel with a detailed graphical analysis based on EXFOR, have been applied stimulating new measurements, significantly increasing the quality of this activation file. The next step is to include the EAF uncertainty data for all channels into JEFF-3.0/A.

#### **INTRODUCTION**

The main overall result of the conversion of EAF [1] into ENDF-6 format [2] is that all reactions are combined into one ENDF-6 formatted file by nucleus and so can be seamlessly used by many evaluators, codes, and applications worldwide. EAF-2003 and JEFF-3.0/A, as the ENDF-6 format conversion is termed, contain neutron data for 98 elements, 774 different target nuclei, including first (m) and second (n) isomeric states, from H-1 to Fm-257, with 12617 neutron-induced reactions below 20 MeV. In contrast, the JEFF-3.0/GP general-purpose transport file contains data for about half that number-340 nuclei. The latter is sufficient for neutron transport calculations following the neutrons and the major target nuclei but not all the daughter products nor the emitted particles. An activation file like JEFF-3.0/A allows codes to follow all the target nucleus states, the incident, and emitted particles (i.e., charged particles, gas production) as well as the residual nucleus states, as a function of time.

#### **ENDF-6 FILE FORMAT**

The JEFF-3.0/A (EAF-2003 into ENDF-6) file layout for each nucleus is as follows:

MI	5 Description
1	General information, comments
2	Resonance parameters, skeleton
3	Total reaction channels
8	Flag, file pointer, dictionary
9	Isomeric branching ratio.
10	Split threshold reaction channels

This layout allows for 23 open reaction channels or MT numbers: 4, 16, 17, 18, 22, 24, 25, 28, 29, 32, 33, 34, 37, 41, 102, 103, 104, 105, 106, 107, 108, 111, and 112, for each nucleus. Each of those channels could be further broken down into three partials leading to the ground, first, and/or second isomeric states of the daughter product. Table 1 describes the relation between MT and reaction type, listing the total number of reactions for each type present in JEFF-3.0/A.

TABLE 1. Reactions types and MTs in JEFF-3.0/A.

Reaction Type (23)	MT	No. of Reactions
(n,n')	4	262
(n,2n)	16	1010
(n,3n)	17	871
(n,f)	18	90
$(n,n'\alpha)$	22	907
(n,2nα)	24	4
(n,3nα)	25	2
(n,n'p)	28	922
$(n,n2\alpha)$	29	1
(n,n'd)	32	904
(n,n't)	33	791
(n,n'h)	34	208
(n,4n)	37	25
(n,2np)	41	7
(n,γ)	102	1007
(n,p)	103	1016
(n,d)	104	927
(n,t)	105	951
(n,h)	106	862
(n,α)	107	992
(n,2α)	108	2
(n,2p)	111	822
(n,pα)	112	34
Total		12617

The translation of EAF into ENDF-6 format is performed with EAF2ENDF, a code originally developed to produce high-energy activation libraries [3]. First of all, an MF-1 is included containing the main information and documentation. The description of MF-3 has been copied directly from the EAF comment lines including the original EAF MTnumbers, data source, relevant comments, and numbers describing the modifications performed on the original evaluation [4].

A trivial MF-2 follows since the original EAF-file does not contain resonance data. Therefore,  $r = 1.35 \times (A^{1/3})$  is computed for the scattering radius and a very small resonance region is used. All the resonant channels (i.e.,  $(n,\gamma)$ , (n,f),  $(n,\alpha)$  and (n,p)) are already stored as PENDF in EAF, which is a linearised pointwise format.

For the storage of activation excitation functions, a combination of MF-3, MF-8, MF-9, and MF-10 is used. In this particular case, file 8 does not describe radioactive decay and fission yield data but, as approved by the members of the Cross Section Evaluation Working Group CSEWG at the November 2001 meeting, nuclide production information. When the reaction populates the ground state only, or when the specific population is unknown, MF-3 is used, as usual. Reactions to isomeric states for threshold reaction channels are stored in MF-10, using the

normal ENDF-6 nomenclature. For the resonant  $(n,\gamma)$  channel, the total reaction is stored in MF-3, MT-102, and the branching ratio in MF-9 when it exists. Furthermore, MF-8 specifies where the (isomeric or nonisomeric) information can be found while including the reaction daughter MAT and ZAm number. Hence, for all MT-numbers, MF-8 always points to either MF-3, MF-9, or MF-10. This also means that MF-3 and MF-10 cannot be populated simultaneously for the same MT-number. Consequently, the total reaction cross section is not stored when the partials exist and vice versa. The ENDF-6 manual [2] should be consulted for further details.

Normally all the original EAF data remain unchanged and only the file format is modified. This is not entirely true, and minor changes can occur when double or very low values are encountered. In EAF format, all isomeric cross sections are explicitly described; however, the ENDF-6 manual requires a branching ratio for all resonant channels, to be accounted for in MF-2 and stored in MF-9. This means that, when required, the partial capture channels have been, first, put on a common energy grid, then summed and their energy-dependent branching ratio calculated, and finally thinned to a 3-digit accuracy. The outcome of these new processes is an MF-9 for 219 reactions, containing capture isomeric-branching ratios leading to the ground, first isomer, and sometimes (18) the second isomer daughter. The information was there, in the original EAF format; however, storage in this ENDF-6 compliant format will facilitate usage of the energy dependence of the nuclear data.

New MAT numbers have been assigned following the strategy used for ENDF/B-VI where the MAT for isotopes of an element are assigned on the basis of increasing mass steps of three, allowing for the ground state and two metastable states:

 $MAT = 100 \times Z + 25 + 3 \times (A-Amin) + isom.$ 

The details of the range of reactions contained in EAF-2003 [1], a full JEFF-3.0/A file index and the MAT number are given in the file documentation.

#### **JEFF-3.0/A VALIDATION**

An important, added bonus of having the EAF-2003 data in ENDF-6 format is that the ENDF suite of utilities and checker codes [5] can be used. Although EAF-2003 has been put through several QA processes in SAFEPAQ-II [4] (file format, C/S and C/E cross-section validations, EXFOR differential graph comparison, etc.) and validated against experimental data with the EASY-2003 code system

and other activation codes, it is an important and required procedure in line with the nuclear data centre QA recommendations. Figures 1 and 2 show typical SAFEPAQ-II validation graphs.



FIGURE 1. C/Experiment of resonance integral.



FIGURE 2. C/Systematic at 14.5 MeV of (n,2n).

Format (CHECKR) and physics checking (FIZCON and PSYCHE) have been performed with version 6.13 of the code on JEFF-3.0/A, and no significant error messages were noted. Some trivial messages tend to occur, but are not of concern for an activation file. One has to remember that JEFF-3.0/A is an activation file, in distinction to the JEFF-3/GP transport file, and so does not need to contain certain physical parameters such as angular distributions, elastic cross sections, emitted particle spectra, or to obey certain ENDF-6 rules.

The other utility codes such as GETMAT, LISTEF, or INTER allow the retrieval of materials, generation of file summary and annotated data listings, or the calculation of selected cross sections and integrals.

Other validation methods rely on plotting the excitation function of the open channel with the differential experimental information stored in the EXFOR database as in Fig. 3.



FIGURE 3. Yttrium inelastic cross section.

The EAF file has been validated using integral data produced from several laboratories (FNG, FNS, SNEG, FZK, TUD, etc.) with diverse neutron fields. In addition, literature data typically produced during the 1970s have been used. These include measurements in the Cf-252 spectrum. Around 300 reactions of JEFF-3.0/A can be scrutinized in such a way [6].

Figure 4 shows the integral C/E results for the Si-29(n,p)Al-29 reaction using data from JEFF-3.0/A. Five independent integral experimental results are compared with calculations using the EASY code package. The points represent the ratio of the EAF value (C) to the measured value (E) for the cross section averaged in the neutron spectrum. The hatched band represents the EAF uncertainty. One can notice that this threshold cross section is well represented in the first four neutron fields. In these the error bars overlap the uncertainty band. This agreement is further endorsed by Fig. 5 in which the excitation function and differential measurements are superposed with their associated uncertainties.

Decay heat measurements of pure material samples irradiated in the JAERI FNS assembly proved to be an additional valuable source of information. Figure 6 shows an example.



FIGURE 4. Integral C/E for Si-29(n,p)Al-29.



FIGURE 5. Si-29(n,p)Al-29 cross section.



FIGURE 6. C/E for Hafnium short time decay heat.

#### FILE PROCESSING

The JEFF-3.0/A file can be processed by the code NJOY-99 [7] (above update 68, in an automatic mode) in contrast to the original EAF-2003 file (in EAF format) that was processed by SAFEPAQ-II for the European Activation System EASY-2003. In the latter, the resulting format of the many original multi-group libraries is the libout format of the code FOUR ACES (ENEA Bologna), with two additional comment lines, copied from the point-wise EAF file for each reaction. Group-wise cross sections may differ slightly, depending on which processing tools and weighting spectra have been used: NJOY-99, CALENDF-2002, PREPRO2002, SAFEPAQ-II etc.

With NJOY-99, from the original 293.6K ENDF-6 format, JEFF-3.0/A files, multiple-temperature PENDF files can be generated with the Doppler-broadening module *broadr*. This step can then be followed by a choice of group processing through the dedicated module *groupr*, producing a GENDF file, and further *matxsr* or *acer* processing, as required.

The 774 single-nucleus files that compose JEFF-3.0/A can be automatically processed with the Unix C-shell script. The only prerequisite is to have access to an NJOY executable.

#### **CONCLUSIONS**

After many years of trials, experiments, and proposals, a consensus has been found on the file format of a large activation file. This format has, for the first time, been fully implemented in the EAF-2003 into ENDF-6 conversion, leading to the production of JEFF-3.0/A and allowing more exact nuclear data file use and further dissemination. This important milestone brings us a step nearer to a universal evaluated nuclear data file format.

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