HEDL-TME 81-31 UC-79d ENDF-316

FTR SET 500, A MULTIGROUP CROSS-SECTION SET FOR FTR ANALYSIS

Hanford Engineering Development Laboratory

HANFORD ENGINEERING DEVELOPMENT LABORATORY Operated by Westinghouse Hanford Company P.O. Box 1970 Richland, WA 99352 A Subsidiary of Westinghouse Electric Corporation Prepared for the U.S. Department of Energy under Contract No. DE-AC06-76FF02170

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F.M. Mann February 1982

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FOR FTR ANALYSIS

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ABSTRACT

FTR Set 500 is a 53-neutron-group, 20-photon-group, cross-section set based on ENDF/B-V cross sections and neutron spectra typical of the Fast Test Reactor (FTR). This report describes the specifications and processing of Set 500 and provides one-group values of this set for use in limited FTR analyses.

ACKNOWLEDGMENTS

The help of R. E. MacFarlane (LANL) in the debugging and operation of his NJOY code is most gratefully noted. His generous shipment of the PENDF tapes greatly reduced computer costs. The efforts of F. Schmittroth in preparing the flux weighting functions and R. E. Schenter for processing and testing the cross sections are also appreciated. The needs of the Core Physics and the Radiation and Shield Analysis groups of the FFTF Project, as determined by discussions with J. A. Rawlins, R. B. Rothrock, and L. L. Carter, helped motivate this work and determine its direction.

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FTR SET 500, A MULTIGROUP CROSS-SECTION SET FOR FTR ANALYSIS

I. SUMMARY

The Fast Test Reactor (FTR) of the Fast Flux Test Facility (FFTF) is designed to test fuels and materials for the US fast breeder program. The FTR, a sodium-cooled, 400-MWt, plutonium-fueled reactor located at the Hanford Engineering Development Laboratory (HEDL) was designed with FTR Set $300^{(1)}$ and $3005^{(2)}$ cross sections that were based on a modification ⁽³⁾ of the second version of the Evaluated Nuclear Data File (ENDF/B-II).

FTR Set 500 is a 53-neutron-group, 20-photon-group, cross-section set based on ENDF/B-V⁽⁴⁾ cross sections and neutron spectra typical of the FTR. This new set incorporates additional information gained since Set 300 was generated and adds nine groups to better represent the high-energy neutron region. In addition, unlike Sets 300 and 300S, Set 500 uses a flux weighting typical of neutron spectra of fast breeder reactors, rather than a 1/E + fission spectrum shape. As Set 500 consists of infinitely dilute cross sections, self-shielding factors, and Pl neutron and photon transfer matrices, diffusion and transport calculations can now be performed based on the same cross sections.

Section II of this report describes the specifications of FTR SET 500, while Section III details the processing methods, and Section IV the results including FTR spectral averaged values. Section V discusses the limitations of this processed data set.

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II. SPECIFICATIONS OF SET 500

A. CROSS-SECTION SOURCE

The source of all unprocessed cross sections used in this work is the fifth version of the Evaluated Nuclear Data File (ENDF/B-V).⁽⁴⁾ ENDF/B-V provides a unified format for the storage and retrieval of evaluated nuclear data. The file including evaluations is overseen by the Cross-Section Evaluation Working Group (CSEWG), which has representatives from the US government, federal laboratories, universities, and industrial firms.

In general, evaluations are based on the latest experimental differential data and on advanced nuclear theories. Each evaluation is reviewed by personnel at a different laboratory than the one at which the evaluation is created. A committee of CSEWG then formally reviews each evaluation and accepts it into the ENDF/B system. After release, the evaluation is further compared with integral benchmark experiments and other appropriate data.

B. MATERIALS

Table 1 displays the materials included in Set 500 along with the evaluators of the ENDF/B-V material. These materials are the minimum necessary for limited FTR analyses; other materials may be added in the future.

Set 500 is based on the self-shielding factor method, (5,6) sometimes called the Bondarenko method. In this method, the weighting flux is modified to account for other materials by the introduction of a background cross section σ_0 (see Section III for more details). Table 1 presents the background cross sections σ_0 for which the various materials were run. The chosen values were based on past FTR calculations.

All materials were processed at two temperatures, 300 K and 1200 K. In addition, the actinide materials were processed at an additional temperature of 2100 K. Again, the values were chosen from past experience.

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CONTENTS OF FTR SET 500*

leference	14	15	16	14	17	18	15	19	20	15	12	22	15	23	23	24
Evaluators (Laboratory)	G.Hale, L.Stewart, P.G.Young (LANL)	C.Cowan (GE-BNL)	C.Y.Fu, F.G.Perey (ORNL)	P.G.Young, D.Foster, Jr., G.Hale (LANL)	D.C.Larson (ORNL)	A.Prince, T.W.Burrows (BNL)	S.F.Mughabghab (BNL)	C.Y.Fu, F.G.Perey (ORNL)	M.Divadeenam (BNL)	R.Howerton (LLNL), F.Schmittroth, R.E.Schenter (HEDL)	M.R.Bhat (BNL)	E.Pennington, A.Smith, W.Poenitz (ANL)	E.Kujawski (GE-FBRD), L.Stewart (LANL)	L.W.Weston (ORNL)	L.W.Weston, R.Q.Wright (ORNL), R.Howerton (LLNL)	R.E.Schenter (HEDL), L.W.Weston (ORNL)
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oss Se											~	~	~			
and Cr											î	Ŷ	î			
Ckgrou				×	×	×	×	×	×	×	×	×	×	×	×	×
E+4	×	×	×	×		×	×			×	×	×	×	×	×	×
E+5														×	×	
81	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
ENDF/B-V MAT No.	1305	1160	1306	1267	1311	1324	1325	1326	1328	1321	1395	1398	1399	1380	1381	1361
Isotope		1 B**	J	160	²³ Na	ر د	иМ _{сс}	Fe***	Ni	Mo	235 _U	2.38 _{U***}	239 _{Pu***}	240 _{Pu}	241 _{Pu}	241 _{Am}
										4		· · , '				

*53 neutron groups x 20 photon groups, flux weighted with FTR core spectrum. **No photon files given. ***Flux weighted with FTR core spectrum and flux typical of FTR reflector region. ,

C. GROUP STRUCTURE

Set 300 is a 30-neutron-group cross-section set extending to 10 MeV. Additional low-energy groups were later added to form the 42-group 300S set to improve the set for shielding applications. To increase the understanding of the high-energy neutron region (especially for passive dosimetry), additional groups were added above 1 MeV and the set now extends to \sim 17 MeV. The resulting 53-group structure (shown in Table 2) provides the basis for Set 500 and is directly collapsible to the 42-group set of 300S.

Unlike earlier FTR cross-section sets, Set 500 contains photon production cross sections. The photon group structure is shown in Table 3.

D. FLUX WEIGHTING

Most multigroup cross-section sets $(^{7,8})$ are reactor-independent and frequently use a 1/E + fission spectrum shape for the slowly varying flux shape. For FTR Set 500, however, two weighting spectra typical of the FTR were used. Both spectra were obtained from 42-group, three-dimensional diffusion calculations made by the HEDL Core Physics group. The midplane flux for the central assembly was selected as a typical core spectrum and was used to weight all cross sections. A limited set of cross sections (Fe, 238 U, 239 Pu) was weighted with the midplane spectrum characteristic of the reflector region. The use of two spectra not only provides more accurate values but also provides the opportunity to judge the importance of the weighting spectrum. Additional weighting spectra (such as $1/E_n$) may also be added in the future.

The next step was the construction of a pointwise representation of the 42-group fluxes shown in Figure 1. Specifically, the flux per unit lethargy $\phi_{II}(E)$ was defined at the midpoint energy E* of each lethargy interval Δu by

$$\phi_u(E^*) = \phi_g / \Delta u$$

where:

 ϕ_{a} = multigroup flux.

TABLE 2

NEUTRON GROUP ENERGIES

Group	Upper Group Energy (eV)	Delta Lethargy	FTR Set 300S
1	1.69046 E+7	0.1250	
2	1.49182 E+7	0.1000	
3.	1.34986 E+7	0.1500	
5	1.00000 E+7	0.1500	х
6	8.60708 E+6	0.1500	
7	7.40818 E+6	0.2000	v
8 9	4.96585 E+6	0.3000	^
10	3.67879 E+6	0.2500	X
11	2.86505 E+6	0.2500	v
12	2.23130 E+6 1 73774 E+6	0.2500	X
14	1.35335 E+6	0.2000	х
15	1.10803 E+6	0.3000	
16	8.20850 E+5	0.2500	X
18	4.97871 F+5	0.2500	x
19	3.87742 E+5	0.2500	x
20	3.01974 E+5	0.5000	X
21	1.83156 E+5	0.5000	X
22	6.73795 E+4	0.5000	Ŷ
24	4.08677 E+4	0.4700	X
25	2.55424 E+4	0.2500	X
26	1.98925 E+4	0.2800	X Y
28	9.11882 E+3	0.5000	â
29	5.53084 E+3	0.5000	X
30	3.35463 E+3	0.1667	X
31	2.83954 E+3 2 40378 F+3	0.1667	X X
33	2.03468 E+3	0.5000	x
34	1.23410 E+3	0.5000	x
35	7.48518 E+2	0.5000	X
30 37	4.53999 E+2 2 75365 E+2	0.5000	x
38	1.67017 E+2	0.5000	x
39	1.01301 E+2	0.5000	X
40	6.14421 E+1 3 72665 E+1	0.5000	X Y
41	2.26033 E+1	0.5000	â
43	1.37096 E+1	0.5000	X
44	8.31529 E+0	0.5000	X
45	5.04348 E+0 3.05002 E+0	0.5000	X
40	1.85539 E+0	0.5000	Ŷ
48	1.12535 E+0	0.5000	X
49	6.82560 E-1	0.5000	X
50	4.13994 E-1	0.5000	X
52	1.52300 E-1	0.5000	X
53	9.23745 E-2	9.1310	X
	1.00000 E-5		

TABLE 3

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PHOTON GROUP ENERGIES

Group	Upper Group Energy (MeV)
uroup	Lifer gy (fier)
1	15.0
2	10.0
3	9.0
4	8.0
5	7.0
6	6.0
7	5.0
8	4.0
9	3.5
10	3.0
11	2.5
12	2.0
13	1.6
14	1.2
15	0.90
16	0.60
17	0.40
18	0.21
19	0.12
20	0.07
	0.01





Values of $\phi_u(E)$ were added at 12.5 MeV and 20.0 MeV based upon the 239 Pu fission spectrum:

$$\phi(E) = C E^{3/2} \exp(-E/1.415 \times 10^6 \text{ eV})$$

where C was chosen to match $\phi_u(E)$ at the highest E* (7.78 MeV) obtained from the 42-group structure. For the lowest energy group (<0.092 eV), a Maxwellian shape with an effective temperature of 0.04 eV (T \sim 500 K) was used. For energies between the specified midpoints (E*), a log-log interpolation in $\phi(E)$ was used.



III. PROCESSING

A. CODES

The commonly used nuclear cross-section processing code at HEDL is ETOX.⁽⁹⁾ However, the NJOY⁽¹⁰⁾ processing code developed by the Los Alamos National Laboratory (LANL) produces not only diffusion cross sections but also transport cross sections, all with arbitrary flux weighting. Thus NJOY was used for all cross-section processing for FTR Set 500.

Figure 2 shows the logic flow for NJOY and related codes. NJOY is a modular code, allowing files to be saved at intermediate steps. The MODER module converts the card image ENDF/B tape into binary format. The RECONR module reconstructs resolved resonance shapes from the resolved parameters. the BROADR module Doppler broadens the cross sections, while UNRESR calculates cross sections from the unresolved resonance parameters. Finally, the HEATR module adds KERMA (Kinetic Energy Release in Material) and displacement cross sections to complete the pointwise ENDF/B (PENDF) tape. LANL supplied various PENDF tapes that are shown in Table 4. The use of these tapes greatly reduces the cost of producing a library as \sim 50% of the computer time is spent in creating the PENDF tapes.

The GROUPR module calculates multigroup cross sections and produces a group ENDF (GENDF) tape. The DTFR module reformats the GENDF tape into a file readable by DTF and similar transport codes. Processing for diffusion codes follows a different path. The CCCCR module produces the standard interface files ⁽¹¹⁾ ISOTXS and BRKOXS as specified by the DOE/RRT Committee for Computer Code Coordination. ISOTXS contains infinitely dilute cross sections, while BRKOXS corrects for temperature and other material factors.

As HEDL does not use standard interface files, two auxiliary codes CINX⁽¹²⁾ and PUPX are used. CINX produces an ETOX-like output, which is labelled FTR Set 500. A modified version of the HEDL library handling code PUPX creates a binary library file readable by a new version of 1DX,⁽¹³⁾ the onedimensional, diffusion-mixing code that starts the HEDL reactor physics calculation sequence.

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HEDL 8109-031.2

FIGURE 2. Logic Flow in NJOY and Related Codes.

TABLE 4

PENDF TAPE DESCRIPTION*

.

	8000											×	×	×	×	×	×
	4000	×	×	×		×	×	~	×	×	×	×	×	×	×	×	×
	2100	×	×			×	×	×	×	×	×	×	×	×	×	×	×
(K)	2000			×													
ature	1200	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
Temper	006	×	×			×	×	×	×	×	×	×	×	×	×	×	×
	808			×													
1	600	×	×	×		×	×	×	×	×	×	×	×	×	×	×	×
	300	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
No. of	Temps	9	9	9	2	9	9	9	9	9	9	7	7	7	7	7	7
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	E										×	×	×	×	×	×	×
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()	<u>1 E+2</u>										×	×	×	×	×	×	×
barns)	<u>3 E+2</u>											×	×	×			
αD	1 E+3										×	×	×	×	×	×	×
	1 E+4										×	×	×	×	×	×	×
	1 E+2														×	×	×
	8										×	×	×	×	×	×	×
No. of	0 S	0	0	0	0	0	0	0	0	0	9	9	7	9	7	7	2
ENDF/B-V	MAT No.	1305	1160	1306	1276	1311	1324	1325	1326	1328	1321	1395	1398	1399	1380	1381	1361
	Isotope	10 ⁸	8	ں ;	091	²³ Na	ۍ ¦	uM ^{c c}	Fe	Ņ	Mo	235 _U	238 ₀	239 _{Pu}	240 _{Pu}	241 _{Pu}	241 _{Am}

*Fractional reconstruction tolerance = 0.005

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B. METHODS

NJOY uses the self-shielding factor (or Bondarenko) method. (5,6) In a resonance region, the neutron flux will be depressed, thereby reducing the contribution of that resonance to the reaction rate. The magnitude of this self-shielding depends in a complex way on the temperature, composition, and geometry of the problem. However, for many problems, accurate reaction rates can be computed using average cross sections defined by

$$\sigma_{\chi \ell g}^{i}(T,\sigma_{0}) = \frac{\int_{g} \sigma_{\chi}^{i}(E,T) \phi_{\ell}^{i}(E,T,\sigma_{0}) dE}{\int_{g} \phi_{\ell}^{i}(E,T,\sigma_{0}) dE}$$

and the weight function for material i is given by

$$\phi_{\ell}^{i}(E,T,\sigma_{O}) = \frac{\phi(E)}{[\sigma_{O} + \sigma_{t}^{i}(E,T)]^{\ell+1}}$$

where:

The file ISOTXS contains "infinite dilution" cross sections at 300 K, $\sigma_0 = \infty$, $\sigma_{\chi \ell g}^{i}$ (T = 300 K, $\sigma_0 = \infty$). Temperature and σ_0 -dependent cross sections are obtained by interpolating in tables of f factors

$$f_{\chi^{\ell g}}^{i}(T,\sigma_{0}) = \frac{\sigma_{\chi^{\ell g}}(T,\sigma_{0})}{\sigma_{\chi^{\ell g}}^{i}(300 \text{ K},\infty)}$$

These are given in the BRKOXS file. Current weighting (l=1) is used for the total cross-section f factor, while flux weighting (l=0) is used for the elastic, capture, and fission cross-section f factors.

Group-to-group transfer matrices at infinite dilution were computed from

$$\sigma_{x^{\ell}g^{\star}g^{\star}g^{\star}}^{i} = \frac{\int_{g} dE \int_{g'} dE' \sigma_{x}^{i}(E) F_{x\ell}^{i}(E^{\star}E') \phi(E)}{\int_{q} \phi(E) dE}$$

where:

g = Initial energy group g' = Final energy group Fⁱ_X(E+E') = Legendre component of the probability of scattering from E to E'

The elastic removal cross section is given by

$$\sigma_{dg}^{i} = \sum_{q' \neq q} \sigma_{eo q \neq q'}^{i}$$

The transport cross section is calculated using

$$\sigma_{\text{tr,g}}^{i}(T,\sigma_{0}) = \sigma_{\text{tlg}}(T,\sigma_{0}) - \sum_{\chi g'} \sigma_{\chi \ell g \neq g'}^{i} (T,\sigma_{0})$$

Note that 1DX calculates σ_{tr} internally.

Finally, the fission chi matrix is given by

$$x_{g \neq g'}^{i} = \frac{\int_{g} dE \int_{g'} dE' v^{i}(E) \sigma_{f}^{i}(E) \chi^{i}(E \neq E') \phi(E)}{\int_{g} dE v'(E) \sigma_{p}^{i}(E) \phi(E)}$$

Since χ^{1}_{g+g} , does not vary much as a function of incoming neutron energy for low energies, the CCCCR module collapses groups 15 + 53 into 1 group.

C. FORMATS

Results of processing are available in the format of the files shown in Figure 2. The main output is shown as FTR Set 500 (the format shown in Table 5). This card image file, which is quite similar to the ETOX output format, contains infinitely dilute cross sections, f factors, and transfer (including χ) matrices and is suitable for diffusion calculations. An alternative representation is also available in the ETOX output format. This representation (in 53 groups or in the 42-group structure of FTR Set 300S) does not contain the χ matrices, elastic down scattering, or removal cross sections.

The DTF format has response function edits of KERMA and σ_{γ} (or σ_{f} for the actinides) as well as the σ_{a} , $v\sigma_{f}$, and σ_{t} standard edits. Complete Pl downscattering and photon production matrices are also given. Infinitely dilute values are given for T = 300 K, 1200 K and (for the actinides) 2100 K, as are values for T = 300 K and σ_{o} = min.

All intermediate files have been saved so that quantities like delayed neutron spectra, which do not have standardized formats, can also be supplied.

TABLE 5

SET 500 FORMAT

NG = Number of groups (53) NX = Number of downscatter and inscatter groups (53) 1. Header Card (A8, A6, E6.2, 916) HOLN = Hollerith descriptor MAT = Material number ATW = Atomic weight (in neutron masses) ICHI = No. of fission groups NT = No. of temperature values NGB = First group having f factors NGE = Last group having f factors NPFF(5) = No. of σ_0 's for fission, capture, elastic, removal, total

2. Temperatures (12F6.0)

(TEM(K), K=1, NT) = temperatures

3. f Factor Block - fission, capture, elastic, removal, total

A. SIGO(6E12.3)

- $(SIGO(K), K=1, NPFF(I)) = \sigma_0$ for Ith reactor B. f factor (I6, (6F12.6)) repeated for each group L = group number
 - ((F(I,J),J=1,NPFF(I)),I=1,NT) = f factor for Ith reactor, Jth temperature

4. Fission Matrix Data

- A. Fission matrix (I6,(6E12.6)) repeated ICHI times
 L = group number
 (CHIISO(L,K),K=1,NG) = fission matrix for group L to
- group K B. Pointer vector (1216) J = dummy (IOSPEC(I),I=1,NG-1) = vector describing collapsing of fission matrix

TABLE 5 (Cont'd)

5. Principal Cross Sections (I6,(6F12.6)) repeated for each group

TRANS = Transport cross section SIGF = Fission cross section YNU = Nu bar = Capture cross section = $\sigma(n,\gamma) + \sigma(n,p) + \sigma(n,\alpha)$ SIGC = Total cross section SIGT SIGEL = Elastic cross section YMUEL = Average cosine for elastic scattering XI = X I SIGDEL = SIG DEL SIGIN = Inelastic cross section [SIGT - SIGEL - SIGC - SIGF $= \sigma(n,n') + \sigma(n,2n) + \sigma(n,3n)]$

6. Inelastic Matrix (I6,(6F12.6)) repeated for each group

L = group number (SM(L,K),K=1,NX) = downscattering from group L to group Kby inelastic scattering $[\sigma_{g^*g'}(n,n') + 2\sigma_{g^*g'}(n,2n) + 3\sigma_{g^*g'}(n,3n)]$

7. Elastic Matrix (I6,(6F12.6)) repeated for each group

L = group number (SE(L,K),K=1,NX) = downscattering from group L to group K by elastic scattering

IV. RESULTS

A. VERIFICATION

As NJOY was a new code to HEDL, its results were verified against values obtained by NJOY at LANL and by ETOX at HEDL. ²³⁸Pu values from LANL were almost identical to values obtained in this study, differing only in the fifth decimal place. As the LANL results were from a CDC 7600, while the HEDL results were from a UNIVAC 1144, this small difference could just be from the different word sizes of the two computers. Results of the LANL NJOY processing for different materials were compared with different codes at ORNL and ANL, and no discrepancies were found.

²³⁹Pu multigroup values calculated by the HEDL code ETOX were identical to the values calculated using NJOY with a 1/E flux weighting. Other specialized codes in use at HEDL showed excellent agreement with the infinitely dilute quantities calculated by NJOY using various flux weightings.

The DTF side of the chain was checked by comparing Monte Carlo results with ANISN runs using similarly prepared cross sections to Set 500.

B. FTR SPECTRAL-AVERAGED VALUES

Table 6 presents spectral-averaged values for the cross sections of Set 500 for two spectra, FTR core center and FTR reflector, based on the core center weighted multigroup cross sections.

TABLE 6

FFTF SPECTRAL-AVERAGED CROSS SECTIONS

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																			0000	inc.											0167	0440	0065	0600	0162	;	
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.t)	5062	:	*	ł	ł	1	*	;	1	1	;	;	I	;	;	1	;		2 1010												2.48 2	2.47 2	.95 2	2.88 2	2.99 2	3.17 3	2015 L
E	2101	:	*	\$;	1	*	1	:	1	1	ł	1	;	;	1	:		000		134	120	113	0871	0599	0254	0250	0264	0229	0146	0055 2	0056 2	0053 2	0053 2	0051 2	0020	016
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V. LIMITATIONS

Although the present cross-section set is adequate for limited FTR analyses, detailed analyses will require more data. Additional materials (such as 232 Th and fission products) are needed for analysis of nonstandard assemblies and full cycle irradiations. Also more materials (besides Fe, 238 U, and 239 Pu) should be weighted with the reflector flux to properly indicate the spectral variation of the FTR.

The present set is heavily biased toward reactor physics calculations. For shielding calculations, the present library is quite limited. Activation cross sections are needed for delayed photon source terms. The photon productions matrices and KERMA factors should be modified to include the decay of short-lived activation products. For the transport of neutrons through shields, a different flux weighting is needed, higher-order scattering moments need to be included, and different materials (e.g., H) need to be added.

Nonetheless, the FTR Set 500 is a major start on a nuclear data library that will allow FTR analyses using the latest available nuclear data evaluation.

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