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Title: ACTI - A MCNP Continuous-Energy Neutron Data Library for Prompt Gamma-Ray Spectroscopy

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ACTI - A MCNP Continuous-Energy Neutron Data Library for Prompt Gamma-Ray Spectroscopy

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ABSTRACT

Prompt gamma-ray spectroscopy is used in a wide variety of applications for determining material compositions. High-quality photon-production data from thermal-neutron capture reactions are essential for these applications. Radiation transport codes, such as MCNP™,[1] are often used to design detector systems, determine minimum detection thresholds, etc. These transport codes rely on evaluated nuclear databases such as ENDF (Evaluated Nuclear Data File)[2] to provide the fundamental data used in the transport calculations. Often the photon-production data from incident neutron reactions in the evaluations are of relatively poor quality.

We have compiled the best experimental data for thermal-neutron capture for the naturally occurring isotopes for elements from H through Zn as well as for ^{70,72,73,74,76}Ge, ^{149}Sm, ^{155,157}Gd, ^{181}Ta and ^{182,183,184,186}W. This compilation has been used to update the ENDF evaluations for ^{1}H, ^{4}He, ^{9}Be, ^{14}N, ^{16}O, ^{19}F, Na, Mg, ^{27}Al, ^{32}S, S, ^{35,37}Cl, K, Ca, ^{45}Sc, Ti, ^{51}V, ^{50,52,53,54}Cr, ^{55}Mn, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu and ^{182,183,184,186}W. In addition, the inelastic cross sections and corresponding secondary-photon distributions were updated for ^{16}O.[3,4,5] Complete new evaluations were submitted to ENDF for ^{35,37}Cl.[6] This document will discuss the evaluation effort and the production of the MCNP data library, ACTI, based on the new evaluations.[7] Data from the ENDF evaluations for $^{28\text{-}30}$Si were also included in the ACTI library for completeness. The silicon evaluations were updated in 1997 and include the latest experimental data for radiative capture.[8] The ACTI data library is compatible with MCNP versions 4C and later.

I. BACKGROUND

The motivation behind this work has been discussed extensively in previous documents.[9,10,11] Prompt gamma-ray spectroscopy is used in a wide variety of applications for determining material compositions. This work was originally begun under the auspices of the Multispectral Neutron Logging project at Los Alamos National Laboratory[12,13] and continued under the ACTI CRADA (Advanced Computational Technology Initiative Cooperative Research and Development Agreement).[14] Our goal for all of these projects is to provide the best prompt gamma-ray data for the ENDF

evaluations and to produce an MCNP data library, ACTI, for prompt gamma-ray applications.

II. COMPILATION OF PROMPT GAMMA-RAY ENERGIES AND INTENSITIES FROM RADIATIVE CAPTURE OF THERMAL NEUTRONS

Complete literature searches were performed for prompt gamma rays from thermal neutron capture through August 2000. We concentrated on the naturally occurring nuclides for elements having Z≤30, but included other important isotopes such as ^{70,72,73,74,76}Ge, ^{149}Sm, ^{155,157}Gd, ^{181}Ta and ^{182,183,184,186}W. In almost all cases, the data adopted were from the paper that was the most complete. For a few isotopes, we adopted evaluations published in the *Nuclear Data Sheets*, especially when numerous data sources were needed to complete the data set for that isotope. In other cases, we used several literature sources to complete the evaluation for a given isotope when published data only covered a part of the gamma-ray energy range. For data sources that we considered secondary in quality or completeness, we usually did not adopt a gamma ray if it was not reported by others or did not fit into the known level scheme for the product nucleus. For several isotopes (e.g., ^{12}C, ^{14}N, ^{19}F, ^{23}Na, and ^{45}Sc), there were several high-quality measurements, and the adopted values were almost always in good agreement with those in the other publications.

If known, we cataloged the levels of the product nucleus involved in the emission of a gamma ray. In a number of cases, usually with older measurements, we used the most recent evaluations of level energies of the product nucleus to determine the energies of the emitted gamma rays. Otherwise, the energies reported by the experiments were adopted.

For the gamma-ray intensities, we usually adopted the reported experimental values. In a few cases, we have applied a multiplication factor to the reported intensities as the intensities reported in the literature had an arbitrary normalization or were normalized to the intensities for another isotope. Some of these experimental data sets had been normalized such that the sum of gamma rays from the capture state or into the ground state was 100%. Others were normalized such that the sum of the energy times intensity divided by S_n, the neutron binding energy, was set equal to 100%. When there were many gamma rays measured down to very low intensities, such normalizations are probably good. However, there were cases, e.g., ^{50}Cr, where we felt that the intensities reported in the literature were improperly normalized. Other measurements from the literature were

used to obtain these multiplication factors. Where intensities had not been reported for the decay of low-energy levels, known branching ratios of gamma rays emitted by such levels were used with the sum of gamma rays decaying into those levels to determine intensities for these missing gamma rays.

The sums of the intensities from the capture state and into the ground state were usually close to 100%. In a few cases, the sum into the ground state is low because there were no reported intensities for very low-energy levels decaying into the ground state, such as for the 14-keV level of ^{57}Fe. In other cases, some of the low-lying levels emit internal-conversion electrons instead of gamma rays. Such electrons were not cataloged and can account for some of the missing intensity.

Table 1 gives a summary of the isotopic data compilation. Definitions of the information contained in the table can be found after the table itself. The compilation was then used to update the corresponding ENDF evaluation for a given nuclide as necessary. Additionally, the isotopic data were combined to produce the elemental spectra and published in reference 11. For the elemental spectra for Z≤30, a total of 9758 gamma rays for 30 elements were adopted.

II. MODIFICATIONS TO THE ENDF EVALUATIONS

The ENDF evaluations continue to be developed under the direction of the Cross Section Evaluation Working Group (CSEWG) that is comprised of representatives from the U.S. Government and industrial laboratories. Since its inception in 1966, CSEWG has improved the evaluated database as new experimental and theoretical information became available, issuing new versions of the ENDF/B library. The present version is Release 8 of the ENDF/B-VI library of evaluations. ENDF/B-VI was originally released in 1990 (Release 0 and 1) and has since been updated 6 times. We used the most recent version of ENDF/B-VI evaluations as the basis for each of our revisions for ^{1}H, ^{4}He, ^{9}Be, ^{14}N, ^{16}O, ^{19}F, Na, Mg, ^{27}Al, ^{32}S, S, K, Ca, ^{45}Sc, Ti, ^{51}V, ^{50,52,53,54}Cr, ^{55}Mn, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu and ^{182,183,184,186}W.

The revised ENDF evaluations were accepted by the Cross Section Evaluation Working Group and are available in Release 8 of ENDF/B-VI. For most of these evaluations, the prompt photon-production data for thermal neutron capture have been modified based on the compilation effort described in Section II. The energy of the gamma-ray from thermal capture by ^{1}H was adjusted from 2.2246 (the Q value) to 2.2233 MeV to take into account

the recoil energy of the product nucleus. The atomic weight ratio, the ratio of the atomic weight of the target to the atomic weight of a neutron, was updated for the ^{4}He evaluation. Inelastic cross-sections and corresponding secondary-photon distributions were updated for the ^{16}O evaluation. For ^{35,37}Cl, complete new ENDF evaluations were submitted and accepted that incorporated the new thermal capture data.

A. Representation of Photon-Production Data in the ENDF Evaluations

ENDF was originally organized to provide nuclear data for the fission-reactor program and the system has evolved to include nuclear cross-section data for all applications. Even with the expanded applications coverage, the primary emphasis is for incident neutron cross sections below 20 MeV with modest attention paid to the secondary gamma-ray distributions from radiative capture.

There are a number of mechanisms by which an evaluator can incorporate secondary energy distributions for gamma rays as a function of incident neutron energy. Gamma-ray spectra that have discrete energies and intensities are usually given in File 12 of an evaluation but can also be given in File 6. When an evaluator has elected to use a histogram representation of the gamma-ray spectra, generally binned in 50-250 keV wide energy bins, the data are most often given in File 15. A few evaluators (e.g. ^{9}Be, ^{19}F,…) choose to use a smaller bin width, approximately 2-10 keV, to try and mimic discrete photons in the File 15 distributions. The evaluator may or may not choose to use an energy-dependent yield as a function of incident neutron energy to properly conserve energy. Figure 1 illustrates the use of a binned photon-production spectrum for thermal-neutron-capture in Fe in the original ENDF evaluation. The gamma-ray spectrum is binned in 50 keV wide energy bins. As is often the case, the same spectrum was used for each isotope of Fe. Note that the ^{56}Fe doublet at 7.6312 and 7.6456 MeV is contained in a single energy bin from 7.60 to 7.65 MeV.

B. Incorporation of Revised Photon-Production Data in the ENDF Evaluations

In general, the number of discrete photons from thermal-neutron-induced radiative capture in File 12 was significantly increased. Continuum distributions were included in several cases - either to reduce the number of discrete photons by combining discrete photon data or to provide data on unresolved or unmeasured photons (from theoretical calculations). In all cases except for ^{14}N, the radiative capture photon angular distributions were assumed isotropic, and the File 14 information was updated to reflect the new number of discrete gamma rays. We preserved all information already present in the previous ENDF/B files,

usually File 15, at incident neutron energies above our evaluations. We updated all Q values in File 3 for MT=102 (radiative capture) using the Audi-Wapstra 1995 mass tables.[15] The Q value for the elemental evaluations was specified to be the cross section *and* atomic fraction weighted Q value at thermal incident-neutron energies.

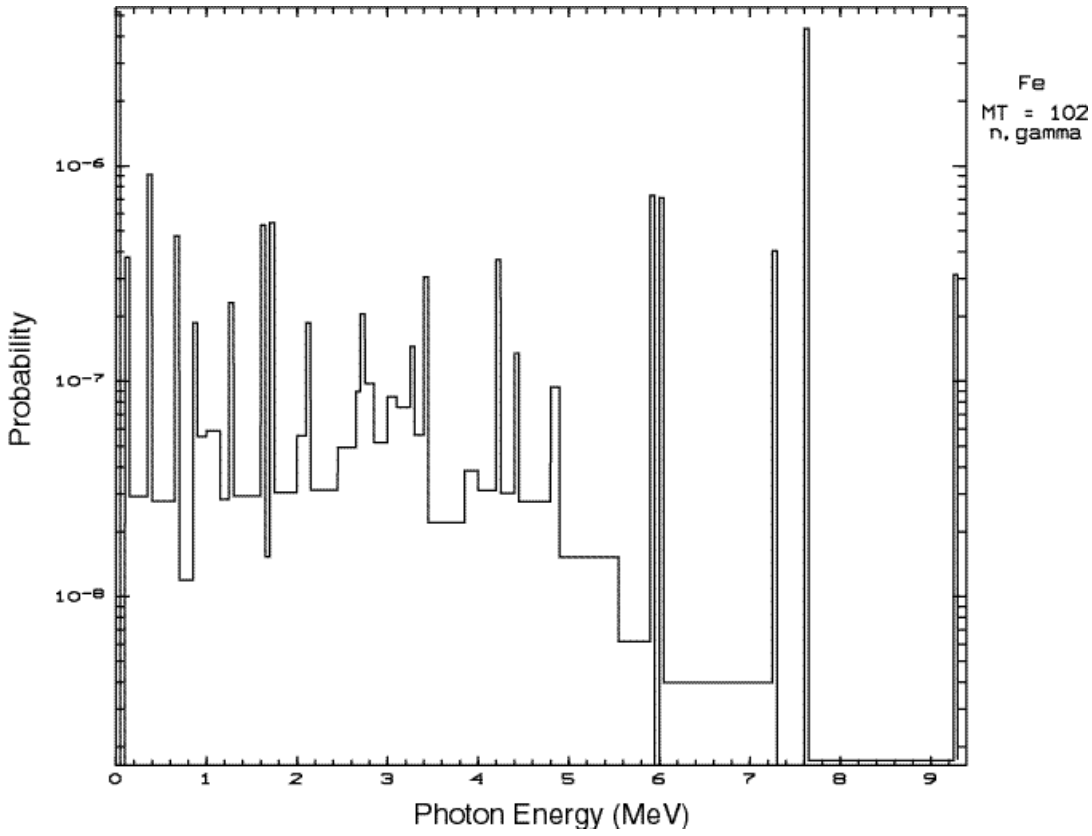

Figure 1. The histogram photon-production spectrum for thermal-neutron capture from the original ENDF evaluations for the iron (Fe) isotopes. The bin width of 50-keV causes the prominent ^{56}Fe doublet at 7.6312-MeV and 7.7456-Mev to be represented as a single peak.

MCNP currently allows a maximum of 1000 discrete photons per nuclide. Elemental evaluations, with contributions from multiple isotopes, can easily exceed this upper limit; for example, natural potassium would have a total of 1741 gamma rays. For these elemental evaluations, we therefore include as discrete gamma rays (in File 12) only those that have an intensity greater than 0.01 times the maximum gamma-ray intensity for that element. The remaining gamma rays are used to form a background continuum spectrum that is included in

the File 15 information. We also used this procedure for individual isotopes that have greater than 600 discrete gamma rays.

To properly conserve energy and ensure more accurate heating numbers, the prompt gamma-ray spectrum was normalized to the total available energy (or Q value) unless a substantial fraction of the gamma-ray spectrum remained unmeasured. In general, normalization factors ranged from 0.9572 to 1.1259, with an average of 1.0107± 0.0204. The spectra remained unnormalized for ^{43}Ca, ^{61}Ni, and ^{182,183,184,186}W, where only 76%, 56%, 55%, 54%, 25%, and 59% of the total spectrum, respectively, was measured. The spectra also remain unnormalized for ^{47,49}Ti because the strongest gamma ray for each isotope would have an unphysical yield if normalized.

The contribution of ^{43}Ca and ^{47,49}Ti to the elemental spectrum was small. For the ^{61}Ni and ^{182,183,184,186}W isotopic evaluations, we used theoretical calculations to estimate the spectrum of unresolved (and unmeasured) gamma rays.
Elemental spectra were constructed from the isotopic evaluated spectra for S, K, Ca, and Ti and were not further normalized. The cross sections and atomic fractions used to construct the elemental spectra were obtained from the Chart of the Nuclides 15th edition.[16] Table 2 gives the representation of the photon production data in the previous ENDF evaluation for radiative capture and the details on the data used to revise the evaluations in this effort. The elemental evaluations for Mg, S, K, Ca, and Ti incorporated 55, 29, 76, 31, and 21 discrete gamma rays respectively. These discrete gamma-rays represented 90.4%, 94.6%, 72.5%, 91.9%, and 90.3% of the total available gamma ray energy.

Detailed information on the changes to each individual evaluation can be found in reference 10. Additionally, information on the gamma-ray energies and intensities for the modified evaluations can be found at:

http://www-xdiv.lanl.gov/PROJECTS/DATA/nuclear/photon/thermal.html

III. CREATION OF THE ACTI LIBRARY

After extensive testing, version 99.50 of the NJOY processing code[17] was used to produce the ACTI library. The ENDF/B-VI release 8 evaluations were processed at temperatures of 77K and 293.6K, and the tungsten isotopes were also processed at 3000K. These processed data can then be used with a new Doppler broadening code to be released in the future through the Radiation Safety Information Computational Center

http://epicws.epm.ornl.gov/rsic.html

The new Doppler broadening code will allow the MCNP user to broaden the data to the temperature of the specific problem they are simulating. As the tungsten evaluations contain unresolved-resonance data, data at the upper temperature limit of 3000K were provided for use with the Doppler broadening code.

The final ACTI data library consists of data for ^{1}H, ^{4}He, ^{9}Be, ^{14}N, ^{16}O, ^{19}F, Na, Mg, ^{27}Al, $^{28\text{-}30}$Si, ^{32}S, S, ^{35,37}Cl, K, Ca, ^{45}Sc, Ti, ^{51}V, ^{50,52,53,54}Cr, ^{55}Mn, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu and ^{182,183,184,186}W . The ACTI library is contained within 2 files, *actia* and *actib*, that are 190Mb and 181Mb in size. The room temperature data can be found in the *actia* file and the 77K and 3000K data can be found in the *actib* file. The ACTI library is compatible with MCNP version 4C. Table 3 contains information for the ACTI Library in a similar form as Appendix G in the MCNP manual. If the data were available in the ENDF evaluation, full charged-particle production information was included in the processing for use with MCNPX.[18] The evaluation date can sometimes be quite misleading. For example, the evaluation portion below an incident-neutron energy of 20 MeV for Ca and the W isotopes dates from 1980 whereas the evaluation above 20 MeV dates from 1996-1997. The evaluation date given in the Appendix G information is the later date of 1996-1997. The File 1 information in each evaluation gives a summary of the history of that evaluation. This information will be located on the WWW at

http://www-xdiv.lanl.gov/PROJECTS/DATA/nuclear/doc/acti.html

A. Testing of the NJOY Processed Files

The Data Team in X-Division at Los Alamos National Laboratory has a suite of 8 ENDF evaluations used to test each version of NJOY. Once a new version of NJOY has been shown to process these evaluations correctly, the processing associated with a specific MCNP data library begins.[19] In addition to the internal consistency checks that NJOY performs,[20] the Data Team has a suite of checking codes that are used to verify each processed file.[21,22,23,24,25] Once this testing process is completed, then each file is run through a standard MCNP run to identify any additional problems.

Modifications were made to the Release 8 ENDF evaluation for ^{45}Sc. It was found in the internal NJOY consistency checks that an incorrect reference frame was specified the secondary neutron distributions for MT=16, 22, 28, and 91. The evaluation was updated to use the proper reference frame for these 4 reactions in the ^{45}Sc evaluation prior to processing. Additionally, ^{45}Sc had another evaluation error for the inelastic photons give in File 13, MT=3. The value for the cross section at the reaction threshold was given

improperly such that the processed data file had a non-zero cross section below the threshold.

On some computing platforms, MCNP compiled in 32-bit mode will fail if it encounters cross sections or distribution values $<10^{-37}$. The exponent for cross-section values $<10^{-37}$ were changed to 10^{-35}. Such low number corrections were made for ^{16}O.

During the final testing of the ACTI library, we discovered that the unresolved-resonance data were not processed as accurately as required for data at multiple temperatures. Additionally, the version of NJOY used for processing did not provide heating numbers in the unresolved-resonance region in the correct units. A patch to NJOY was developed to correct the problem for processing at multiple temperatures. The heating numbers were corrected after processing. These two problems only affected the data for the W isotopes.

B. Gamma-Ray Energies and Intensities in the ACTI Data Library

Information on the discrete photon production in the MCNP neutron data libraries for gamma-ray spectroscopy applications is available on the WWW at:

http://www-xdiv.lanl.gov/PROJECTS/DATA/nuclear/photon/photon.html

A file containing the information on the DISCrete Energy GAMma-rays (DISCEGAM) is available for each MCNP library as appropriate.[26] There are three tables in each DISCEGAM file. The first, and largest, table is an isotope-by-isotope listing of discrete neutron-induced gamma rays. The second table is a compilation of all of the lines from all of the isotopes in the library, listed in ascending order of gamma-ray energy. The last table is simply a list of total neutron cross sections and total photon-production cross sections. The data in each table are given at three incident-neutron energies: 2.53E-8 MeV (labeled "thermal"), 1 MeV, and 14 MeV.

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Table 1. Summary Information for the Compilation of Prompt Gamma Rays from Thermal Neutron Capture for Z ≤ 30

Isotope	N_γ	S_n (keV)	$\frac{\sum E_\gamma I_\gamma}{S_n}$	$\sum I_\gamma$(cs) (%)	$\sum I_\gamma$(gs) (%)	I_γ(max) (%)	I_γ(min) (%)
^{1}H	1	2224.6	100	100	100	100	100
^{2}H	1	6257.3	100	100	100	100	100
^{6}Li	3	7250.0	100	100	100	62	38
^{7}Li	3	2032.8	100	100	100	89.4	10.6
^{9}Be	11	6812.3	100	100	100	65.5	0.05
^{10}B	8	11454.1	101	100	103	65.7	4.7
^{12}C	6	4946.3	100	100	100	67.5	0.16
^{13}C	7	8176.4	100	100	100	84	2.5
^{14}N	58	10833.3	100	101	99	29.9	0.007
^{16}O	4	4143.3	100	100	100	100	18
^{17}O	10	8044.4	78	49	100	100	9.3
^{19}F	168	6601.4	100	100	100	37.9	0.021
^{20}Ne	28	6761.1	94	99	96	73.8	0.114
^{21}Ne	9	10364.0	109	86	100	100	15.6
^{22}Ne	23	5200.6	101	81	104	75	1
^{23}Na	292	6959.4	103	101	99	91.9	0.002
^{24}Mg	33	7330.7	101	100	99	75.8	0.037
^{25}Mg	212	11093.1	99	99	100	93	0.02
^{26}Mg	35	6443.4	100	101	99	65.5	0.051
^{27}Al	280	7725.0	100	102	101	29.7	0.01
^{28}Si	46	8473.5	100	100	100	70.2	0.012
^{29}Si	107	10609.2	98	98	100	45.6	0.034
^{30}Si	33	6587.4	101	101	100	88.2	0.028
^{31}P	214	7935.6	102	97	99	46	0.02
^{32}S	103	8641.6	100	99	98	66.6	0.004
^{33}S	271	11416.9	89	83	100	70	0.003
^{34}S	59	6985.8	96	96	100	55.4	0.016
^{36}S	15	4303.6	101	101	96	93.5	0.522
^{35}Cl	403	8579.7	99	99	100	27.2	0.002
^{37}Cl	79	6107.8	100	91	100	29	0.101
^{36}Ar	28	8788.9	91	93	93	47.5	0.2
^{40}Ar	35	6098.7	100	100	106	76.1	0.03

Table 1 continued

Isotope	N_γ	S_n (keV)	$\frac{\sum E_\gamma I_\gamma}{S_n}$	$\sum I_\gamma$(cs) (%)	$\sum I_\gamma$(gs) (%)	I_γ(max) (%)	I_γ(min) (%)
^{39}K	432	7799.5	101	89	100	86.2	0.009
^{40}K	586	10095.2	100	88	105	40.5	0.001
^{41}K	723	7533.8	100	93	105	32.9	0.005
^{40}Ca	42	8362.7	100	101	100	88.5	0.1
^{42}Ca	63	7933.0	99	99	99	58	0.2
^{43}Ca	279	11132.0	76	49	101	97	0.03
^{44}Ca	51	7414.8	101	100	98	77	0.1
^{46}Ca	10	7276.1	98	100	98	98	0.8
^{48}Ca	3	5146.6	100	100	100	75.5	24.5
^{45}Sc	480	8760.6	104	99	86	28.3	0.01
^{46}Ti	30	8877.7	91	85	110	60	0.6
^{47}Ti	219	11626.6	87	74	100	95.5	0.032
^{48}Ti	97	8142.4	99	99	101	85.5	0.018
^{49}Ti	124	10939.1	93	83	100	99	0.077
^{50}Ti	16	6372.3	95	100	82	41.7	0.8
^{50}V	368	11051.3	91	75	114	80	0.01
^{51}V	306	7311.2	98	96	41	28.1	0.01
^{50}Cr	71	9261.6	85	84	81	68	0.042
^{52}Cr	11	7939.2	94	93	97	58.4	0.4
^{53}Cr	89	9719.0	97	96	100	78.6	0.02
^{54}Cr	85	6246.3	98	90	101	55.5	0.03
^{55}Mn	321	7270.5	103	98	67	36	0.01
^{54}Fe	42	9297.9	103	97	89	66	0.103
^{56}Fe	252	7646.0	100	96	36	29	0.01
^{57}Fe	99	10044.5	97	95	107	66	0.03
^{58}Fe	139	6580.9	100	92	99	59	0.04
^{59}Co	349	7491.9	90	90	91	48	0.02
^{58}Ni	243	8999.4	98	98	96	50.1	0.002
^{60}Ni	142	7820.0	98	99	67	53.3	0.004
^{61}Ni	77	10597.2	56	43	101	76	0.04
^{62}Ni	92	6837.9	100	100	94	84.5	0.006
^{64}Ni	33	6098.0	100	100	36	67	0.06
^{63}Cu	323	7916.0	100	99	96	33.1	0.011
^{65}Cu	424	7065.9	100	93	105	41	0.022

Table 1 continued

Isotope	N_γ	S_n (keV)	$\frac{\sum E_\gamma I_\gamma}{S_n}$	$\sum I_\gamma$(cs) (%)	$\sum I_\gamma$(gs) (%)	I_γ(max) (%)	I_γ(min) (%)
^{64}Zn	57	7979.6	95	96	35	47.8	0.3
^{66}Zn	20	7052.2	91	86	86	54.2	0.9
^{67}Zn	446	10198.2	75	41	97	75	0.005
^{68}Zn	29	6482.2	57	56	72	23.5	0.5

Isotope	Symbol (mass and element symbol) of neutron-capturing isotope.
N_γ	Number of prompt gamma rays adopted for that isotope.
S_n	Neutron separation energy (in keV).
$\sum E_\gamma I_\gamma / S_n$	Sum of the product of the adopted gamma-ray energy E_γ (in keV) times its intensity I_γ (in %) divided by S_n (in keV).
$\sum I_\gamma$(cs)	Sum of the adopted intensities (in %) for known decays from the capturing state (cs).
$\sum I_\gamma$(gs)	Sum of the adopted intensities (in %) for known decays into the ground state.
I_γ(max)	Highest adopted gamma-ray intensity (in %).
I_γ(min)	Lowest adopted gamma-ray intensity (in %).

Table 2. Isotopic Gamma-ray Data in the Revised ENDF Evaluations

Evaluation		Number of Gamma Rays	Q-Value (MeV)	Measured Total Energy (MeV)	Normalization Factor
^{1}H		1	2.2246	2.2233	-
^{9}Be		11	6.81238	6.8253	0.9981
^{14}N		58	10.83339	10.8236	1.0009
^{19}F		168	6.60137	6.6053	0.9994
^{23}Na		292	6.95949	7.2007	0.9665
Mg-nat		55	8.41054	(90.4%)	
	^{24}Mg	***33***	***7.33073***	***7.3879***	***0.9923***
	^{25}Mg	***212***	***11.09316***	***10.9719***	***1.0111***
	^{26}Mg	***35***	***6.44340***	***6.4149***	***1.0044***
^{27}Al		280	7.72511	7.7515	0.9966
^{32}S		103	8.64165	8.6152	1.0031
S - nat		29	8.60238	(94.6%)	-
	^{32}S	***103***	***8.64165***	***8.6152***	***1.0031***
	^{33}S	***271***	***11.41703***	***10.1399***	***1.1259***
	^{34}S	***59***	***6.98590***	***6.7184***	***1.0398***
	^{36}S	***15***	***4.30462***	***4.3425***	***0.9911***
^{35}Cl		403	8.57968	8.5438	1.0070
^{37}Cl		79	6.10783	6.0779	1.0049
K - nat		76	7.79080	(72.5%)	
	^{39}K	***432***	***7.79956***	***7.8629***	***0.9919***
	^{40}K	***586***	***10.09526***	***10.0935***	***1.0002***
	^{41}K	***723***	***7.53383***	***7.5061***	***1.0037***
Ca - nat		31	8.35632	(91.9%)	
	^{40}Ca	***42***	***8.36277***	***8.3417***	***1.0025***
	^{42}Ca	***63***	***7.93306***	***7.8775***	***1.0071***
	^{43}Ca	***279***	***11.13206***	***8.4454***	***----***
	^{44}Ca	***51***	***7.41483***	***7.4594***	***0.9940***
	^{46}Ca	***10***	***7.27617***	***7.1459***	***1.0182***
	^{48}Ca	***3***	***5.14667***	***5.1466***	***1.00002***
^{45}Sc		480	8.76069	9.1524	0.9572

Table 2 Continued

Evaluation		Number of Gamma Rays	Q-Value (MeV)	Measured Total Energy (MeV)	Normalization Factor
Ti - nat		21	8.27195	(90.3%)	
	^{46}Ti	***30***	***8.87778***	***8.0399***	***1.1042***
	^{47}Ti	***219***	***11.62669***	***10.0915***	***----***
	^{48}Ti	***97***	***8.14243***	***8.0746***	***1.0084***
	^{49}Ti	***124***	***10.93922***	***10.1812***	***----***
	^{50}Ti	***16***	***6.37238***	***6.0608***	***1.0514***
^{51}V		306	7.31130	7.1328	1.0250
^{50}Cr		71	9.26170	9.2358	1.0028
^{52}Cr		11	7.93923	7.4672	1.0632
^{53}Cr		89	9.71909	9.3985	1.0341
^{54}Cr		85	6.24635	6.1226	1.0202
^{55}Mn		321	7.27055	7.4598	0.9746
^{54}Fe		42	9.29800	9.5865	0.9699
^{56}Fe		252	7.64609	7.4515	1.0016
^{57}Fe		99	10.04454	10.0316	1.0262
^{58}Fe		139	6.58096	6.5783	1.0013
^{58}Ni		243	8.99951	8.8421	1.0189
^{60}Ni		142	7.82005	7.6757	1.0194
^{61}Ni		77	10.59733	5.9117	----
^{62}Ni		92	6.83791	6.8612	0.9966
^{64}Ni		33	6.09806	6.1176	0.9967
^{63}Cu		322	7.91602	7.9165	0.9998
^{65}Cu		424	7.06599	7.0649	1.0003
^{182}W		446	6.19074	3.4141	----
^{183}W		269	7.41180	3.9962	----
^{184}W		87	5.75378	1.4661	----
^{186}W		533	5.46675	3.2479	----

Table 3. Appendix G.2 Entries for the ACTI Library

ZAID	AWR	Library Name	Source	Org. Eval. Date.	Temp. (K)	Length (words)	Number Energies	Emax (MeV)	GPD	Nu-bar	CP	DN	UR
1001.62c	0.9992	actia	ENDF/B-VI.8	1999	293.6	10128	688	150	yes	no	yes	no	no
2004.62c	3.9682	actia	ENDF/B-VI.8	1973	293.6	5524	588	20	no	no	no	no	no
4009.62c	8.9348	actia	ENDF/B-VI.8	1986	293.6	115407	514	20	yes	no	yes	no	no
7014.62c	13.8828	actia	ENDF/B-VI.8	1997	293.6	145340	1824	150	yes	no	yes	no	no
8016.62c	15.8575	actia	ENDF/B-VI.8	1996	293.6	407432	2759	150	yes	no	yes	no	no
9019.62c	18.8350	actia	ENDF/B-VI.8	1990	293.6	127005	1888	20	yes	no	yes	no	no
11023.62c	22.7920	actia	ENDF/B-VI.8	1977	293.6	69562	3239	20	yes	no	no	no	no
12000.62c	24.0963	actia	ENDF/B-VI.8	1978	293.6	68746	3172	20	yes	no	no	no	no
13027.62c	26.7497	actia	ENDF/B-VI.8	1997	293.6	220418	3081	150	yes	no	yes	no	no
13027.92c	26.7497	actia	ENDF/B-VI.8 [a]	1997	293.6	220449	3081	150	yes	no	yes	no	no
14028.62c	27.7370	actia	ENDF/B-VI.6	1997	293.6	263728	7364	150	yes	no	yes	no	no
14029.62c	28.7280	actia	ENDF/B-VI.8	1997	293.6	252591	4869	150	yes	no	yes	no	no
14030.62c	29.7160	actia	ENDF/B-VI.6	1997	293.6	195852	5781	150	yes	no	yes	no	no
16000.62c	31.7888	actia	ENDF/B-VI.8	1979	293.6	160505	10272	20	yes	no	no	no	no
16032.62c	31.6970	actia	ENDF/B-VI.8	1977	293.6	16050	993	20	yes	no	no	no	no
17035.62c	34.6684	actia	ENDF/B-VI.8	2001[b]	293.6	311841	6987	20	yes	no	yes	no	no
17037.62c	36.6483	actia	ENDF/B-VI.8	2001[b]	293.6	137404	3425	20	yes	no	yes	no	no
19000.62c	38.7660	actia	ENDF/B-VI.8	1967	293.6	52304	2734	20	yes	no	no	no	no
20000.62c	39.7360	actia	ENDF/B-VI.8	1997[c]	293.6	187296	4344	150	yes	no	yes	no	no
21045.62c	44.5679	actia	ENDF/B-VI.8:X	1992	293.6	267570	22382	20	yes	no	no	no	no
22000.62c	47.4676	actia	ENDF/B-VI.8	1977	293.6	125641	10859	20	yes	no	no	no	no
23000.62c	50.5040	actia	ENDF/B-VI.8	1988	293.6	198692	10393	20	yes	no	no	no	no
24050.62c	49.5170	actia	ENDF/B-VI.8	1997	293.6	390799	28138	150	yes	no	yes	no	no
24052.62c	51.4940	actia	ENDF/B-VI.8	1997	293.6	342461	20849	150	yes	no	yes	no	no
24053.62c	52.4860	actia	ENDF/B-VI.8	1997	293.6	287642	13657	150	yes	no	yes	no	no
24054.62c	53.4760	actia	ENDF/B-VI.8	1997	293.6	260423	13593	150	yes	no	yes	no	no
25055.62c	54.4661	actia	ENDF/B-VI.8	1988	293.6	272554	11114	20	yes	no	yes	no	no
26054.62c	53.4760	actia	ENDF/B-VI.8	1996	293.6	311639	19262	150	yes	no	yes	no	no
26056.62c	55.4540	actia	ENDF/B-VI.8	1996	293.6	466257	25606	150	yes	no	yes	no	no
26057.62c	56.4460	actia	ENDF/B-VI.8	1996	293.6	318268	14266	150	yes	no	yes	no	no
26058.62c	57.4360	actia	ENDF/B-VI.8	1989	293.6	165829	11111	20	yes	no	yes	no	no
28058.62c	57.4380	actia	ENDF/B-VI.8	1997	293.6	617974	39020	150	yes	no	yes	no	no

ZAID	AWR	Library Name	Source	Org. Eval. Date.	Temp. (K)	Length (words)	Number Energies	Emax (MeV)	GPD	Nu-bar	CP	DN	UR
28060.62c	59.4160	actia	ENDF/B-VI.8	1997	293.6	407398	21131	150	yes	no	yes	no	no
28061.62c	60.4080	actia	ENDF/B-VI.8	1997	293.6	247188	7379	150	yes	no	yes	no	no
28062.62c	61.3960	actia	ENDF/B-VI.8	1997	293.6	234511	9168	150	yes	no	yes	no	no
28064.62c	63.3790	actia	ENDF/B-VI.8	1997	293.6	198313	7894	150	yes	no	yes	no	no
29063.62c	62.3890	actia	ENDF/B-VI.8	1998	293.6	335072	22892	150	yes	no	yes	no	no
29065.62c	64.3700	actia	ENDF/B-VI.8	1998	293.6	296916	17593	150	yes	no	yes	no	no
74182.62c	180.3900	actia	ENDF/B-VI.8	1996 [b]	293.6	258342	16815	150	yes	no	yes	no	yes
74183.62c	181.3800	actia	ENDF/B-VI.8	1996 [b]	293.6	224856	13086	150	yes	no	yes	no	yes
74184.62c	182.3700	actia	ENDF/B-VI.8	1996 [b]	293.6	194523	10107	150	yes	no	yes	no	yes
74186.62c	184.3600	actia	ENDF/B-VI.8	1996 [b]	293.6	202211	10833	150	yes	no	yes	no	yes
12000.61c	24.0963	actib	ENDF/B-VI.8	1978	77	69108	3213	20	yes	no	no	no	no
13027.61c	26.7497	actib	ENDF/B-VI.8	1997	77	220073	3038	150	yes	no	yes	no	no
13027.91c	26.7497	actib	ENDF/B-VI.8 [a]	1997	77	220104	3038	150	yes	no	yes	no	no
14028.61c	27.7370	actib	ENDF/B-VI.6	1997	77	264592	7472	150	yes	no	yes	no	no
14029.61c	28.7280	actib	ENDF/B-VI.8	1997	77	252671	4879	150	yes	no	yes	no	no
14030.61c	29.7160	actib	ENDF/B-VI.6	1997	77	196252	5831	150	yes	no	yes	no	no
16000.61c	31.7888	actib	ENDF/B-VI.8	1979	77	162749	10459	20	yes	no	no	no	no
16032.61c	31.6970	actib	ENDF/B-VI.8	1977	77	14930	885	20	yes	no	no	no	no
17035.61c	34.6684	actib	ENDF/B-VI.8	2001 [b]	77	316441	7217	20	yes	no	yes	no	no
17037.61c	36.6483	actib	ENDF/B-VI.8	2001 [b]	77	137963	3495	20	yes	no	yes	no	no
20000.61c	39.7360	actib	ENDF/B-VI.8	1997	77	185636	4178	150	yes	no	yes	no	no
22000.61c	47.4676	actib	ENDF/B-VI.8	1977	77	131345	11427	20	yes	no	no	no	no
24050.61c	49.5170	actib	ENDF/B-VI.8	1997	77	405367	29959	150	yes	no	yes	no	no
24052.61c	51.4940	actib	ENDF/B-VI.8	1997	77	344811	21143	150	yes	no	yes	no	no
24053.61c	52.4860	actib	ENDF/B-VI.8	1997	77	292322	14242	150	yes	no	yes	no	no
24054.61c	53.4760	actib	ENDF/B-VI.8	1997	77	262192	13814	150	yes	no	yes	no	no
25055.61c	54.4661	actib	ENDF/B-VI.8	1988	77	279378	11967	20	yes	no	yes	no	no
26054.61c	53.4760	actib	ENDF/B-VI.8	1996	77	318575	20129	150	yes	no	yes	no	no
26056.61c	55.4540	actib	ENDF/B-VI.8	1996	77	475976	26821	150	yes	no	yes	no	no
26057.61c	56.4460	actib	ENDF/B-VI.8	1996	77	319262	14390	150	yes	no	yes	no	no
26058.61c	57.4360	actib	ENDF/B-VI.8	1989	77	169389	11556	20	yes	no	yes	no	no
28058.61c	57.4380	actib	ENDF/B-VI.8	1997	77	630981	40646	150	yes	no	yes	no	no
28060.61c	59.4160	actib	ENDF/B-VI.8	1997	77	424742	22574	150	yes	no	yes	no	no
28061.61c	60.4080	actib	ENDF/B-VI.8	1997	77	247660	7438	150	yes	no	yes	no	no
28062.61c	61.3960	actib	ENDF/B-VI.8	1997	77	234983	9227	150	yes	no	yes	no	no
28064.61c	63.3790	actib	ENDF/B-VI.8	1997	77	199097	7992	150	yes	no	yes	no	no

ZAID	AWR	Library Name	Source	Org. Eval. Date.	Temp. (K)	Length (words)	Number Energies	Emax (MeV)	GPD	Nu-bar	CP	DN	UR
29063.61c	62.3890	actib	ENDF/B-VI.8	1998	77	348384	24556	150	yes	no	yes	no	no
29065.61c	64.3700	actib	ENDF/B-VI.8	1998	77	304772	18575	150	yes	no	yes	no	no
74182.61c	180.3900	actib	ENDF/B-VI.8	1996 [b]	77	269718	18237	150	yes	no	yes	no	yes
74183.61c	181.3800	actib	ENDF/B-VI.8	1996 [b]	77	235761	14449	150	yes	no	yes	no	yes
74184.61c	182.3700	actib	ENDF/B-VI.8	1996 [b]	77	200883	10902	150	yes	no	yes	no	yes
74186.61c	184.3600	actib	ENDF/B-VI.8	1996 [b]	77	207824	11635	150	yes	no	yes	no	yes
74182.63c	180.3900	actib	ENDF/B-VI.8	1996 [b]	3000	232047	13528	150	yes	no	yes	no	yes
74183.63c	181.3800	actib	ENDF/B-VI.8	1996 [b]	3000	198226	9757	150	yes	no	yes	no	yes
74184.63c	182.3700	actib	ENDF/B-VI.8	1996 [b]	3000	181213	8443	150	yes	no	yes	no	yes
74186.63c	184.3600	actib	ENDF/B-VI.8	1996 [b]	3000	190276	9128	150	yes	no	yes	no	yes

[a] The delayed gamma-ray at an energy of 1.7791 MeV from the reaction n+27Al->28Al has been included in the thermal capture photon-production data.
[b] New evaluations for ENDF/B-VI.
[c] Examples of evaluations that have a significantly older date for evaluated data with incident neutron energies below 20 MeV.

Description of Terms:

ZAID - The ZAID is the nuclide identification number with the form
ZZAAA.NNc or ZZAAA.NNd ,
where ZZ is the atomic number, AAA is the mass number (000 for naturally occurring elements), NN is the neutron cross-section set identifier, and c or d indicates continuous energy or discrete reaction data respectively.

Atomic Wt. Ratio: The atomic weight ratio (AWR) is the ratio of the atomic mass of the nuclide to a neutron. This is the AWR that is contained in the original evaluation and that was used in the NJOY processing of the evaluation.

Library - Library that contains the data file for that ZAID.

Source - Indicates the originating evaluation for that data file.
ENDF/B-V.0 or ENDF/B-VI are the evaluated nuclear data files, a US effort coordinated by the National Nuclear Data Center at Brookhaven National Laboratory. The evaluations are updated periodically by evaluators from all over the country, and the release number of the evaluation is given. This is not necessarily the same as the ENDF revision number for that evaluation. For example, Pu-242 is noted as ENDF/B-VI.2 as it is from release 2 of ENDF/B-VI, but it is revision 1 of that evaluation.

----:X - indicates the original evaluation has been modified by the Los Alamos National Laboratory group X-5.

Org. Eval. Date - Indicates the year that the original ENDF evaluation was completed or accepted prior to the modificatiosn described in this paper.

Temp. - Indicates the temperature (°K) at which the data were processed. The temperature enters into the processing of the evaluation into a data file only through the Doppler broadening of cross sections. The user must be aware that without the proper use of the TMP card, MCNP will attempt to correct the data libraries to the default 293.6 °K by modifying the elastic and tot cross sections only.
Doppler broadening refers to a change in cross section resulting from thermal motion (translation, rotation, and vibration) of nuclei in a target material. Doppler broadening is done on all cross sections for incident neutron (nonrelativistic energies) on a target at some temperature (temp) in which the free-atom approximation is valid. In general, an increase in the temperature of the material containing neutron-absorbing nuclei in a homogeneous system results in Doppler broadening of resonances and an increase in resonance absorption. Furthermore, a constant cross section at zero degrees goes to 1/v behavior as the temperature increases. You should not only employ the best evaluations, but also employ evaluations that are at temperaturesa approximating temperatures in your application.

Length - The tot length of a particular cross-section file in words. It is understood that the actual storage requirement in an MCNP problem will often be less because certain data that are unneeded for a problem may be expunged.

Num. of En. - The number of energy points on the grid used for the neutron cross sections for that data file. In general, a finer energy grid (or greater the number of points) indicates a more accurate representation of the cross sections, particularly through the resonance region.

Emax - The maximum incident neutron energy for that data file. For all incident neutron energies greater than Emax, MCNP assumes the last cross section value given.

GPD - 'yes' means that photon-production data are present; 'no' means that such data are not present.

Nubar - for fissionable material, nubar indicates the type of fission nu data available. 'pr' means that only pr nu data are given; 'tot' means that only tot nu data are given; 'both' means that pr and tot nu are given.

CP - 'yes' means that secondary charged-particle data are present; 'no' means that such data are not present.

DN - 'yes' means that delayed neutron data are present; 'no' means that such data are not present.

UR - "yes" means that unresolved resonance data are present; "no" means that such data are not present.