Los Alamos
NATIONAL LABORATORY

memorandum

Applied Physics Division
Diagnostic Applications, X-5
Los Alamos, New Mexico 87545

To/MS: Distribution
From/MS: S. Frankle, X-5 / MS F663
R. Reedy, NIS-2 / MS D436
Phone/FAX: 5-6461 / 5-5553
Symbol: X-5:SCF-01-105(U)
Date: August 31, 2001

SUBJECT: Archive of Evaluated Data for Prompt Gamma-rays from Radiative Capture of Thermal Neutrons

The motivation behind this work has been discussed extensively in previous documents.[1-5] 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 and continued under the ACTI CRADA (Advanced Computational Technology Initiative Cooperative Research and Development Agreement).[6] Our goal for all of these projects was to provide the best prompt gamma-ray data for the ENDF evaluations used to produce data libraries for transport codes such as MCNP.[7]

The dominant need for these applications is for the energies and absolute intensities of the gamma rays made by thermal-neutron capture by the common elements in nature, those with Z = 30. This mass region is also one where existing compilations for such gamma rays have not been revised for some time. Over the past few years, we have compiled isotopic gamma-ray energies and absolute intensities for the capture of thermal neutrons by the elements from hydrogen to zinc as well as ^{70,72,73,74,76}Ge, ^{149}Sm, ^{155,157}Gd, ^{181}Ta, and ^{182,183,184,186}W *from the published literature*. The isotopic data for Z=30 were then combined to form elemental spectra and will be published in Atomic Data and Nuclear Data Tables.[8]

The isotopic spectra were also used to update the Evaluated Nuclear Data File (ENDF/B-VI)[9] Release 6 evaluations for the following nuclides: ^{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. For most of these nuclides, the photon-production data for thermal-neutron capture have been modified. 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 that incorporated revised thermal capture data. The gamma-ray spectra were generally normalized to the available energy for the ENDF modifications. The ENDF modifications are described in detail in the LANL report LA-13812.[10]

The purpose of this memorandum is to document the archive of the evaluated isotopic and elemental data from this effort, as well as the normalized data used to update

ENDF. The archive resides on HPSS under the */hpss/nucldata/mc/special/acti/data* directory. Three subdirectories, *isotopic*, *element*, and *endf*, contain the isotopic, elemental, and ENDF data respectively. It is anticipated that all files under */hpss/nucldata/mc/special/acti* will be archived on CD/DVD and removed from HPSS at some point in the future.

Archive of Evaluated Isotopic and Elemental Data from the Published Literature

The file naming convention used for the isotopic data is *ZZEEAA* where *ZZ* is the atomic number, *EE* is the elemental symbol, and *AA* is the isotopic number for a given nuclide. An example for ^{12}C would be the filename '06c12'. The file naming convention for the elemental data is *ZZEE*, with the same definitions as before. There is a text file under each subdirectory that contains information for the tables of data that are included for each isotope or element in the archive, *isotopic.txt* and *element.txt*. These text files are given in this memorandum as Appendices A and C along with example data files in Appendices B and D respectively. Additionally, there is a summary file in each subdirectory, *isotopic.sum* and *element.sum*, that gives a one line summary of the data for each nuclide. A listing of the subdirectories current contents is given below.

```
/hpss/nucldata/mc/special/acti/data/isotopic
01h1          11na23        18ar36        22ti49        28ni60        62sm149
01h2          12mg24        18ar40        22ti50        28ni61        64gd155
03li6         12mg25        19k39         23v50         28ni62        64gd157
03li7         12mg26        19k40         23v51         28ni64        73ta181
04be9         13al27        19k41         24cr50        29cu63        74w182
05b10         14si28        20ca40        24cr52        29cu65        74w183
06c12         14si29        20ca42        24cr53        30zn64        74w184
06c13         14si30        20ca43        24cr54        30zn66        74w186
07n14         15p31         20ca44        25mn55        30zn67        isotopic.sum
08o16         16s32         20ca46        26fe54        30zn68        isotopic.txt
08o17         16s33         20ca48        26fe56        32ge70
09f19         16s34         21sc45        26fe57        32ge72
10ne20        16s36         22ti46        26fe58        32ge73
10ne21        17cl35        22ti47        27co59        32ge74
10ne22        17cl37        22ti48        28ni58        32ge76

/hpss/nucldata/mc/special/acti/data/element
01h          08o          14si         20ca         26fe         62sm
03li         09f          15p          21sc         27co         64gd
04be         10ne         16s          22ti         28ni         73ta
05b          11na         17cl         23v          29cu         74w
06c          12mg         18ar         24cr         30zn         element.sum
07n          13al         19k          25mn         32ge         element.txt
```

Archive of Data used in the ENDF Modifications

The data used in the ENDF modifications are available in two places; the HPSS directory */hpss/nucldata/mc/special/acti/data/endf* and the WWW at

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

In general, the evaluated data from the published literature were *normalized* to the available energy to ensure that heating calculations with codes such as MCNP are as accurate as possible. Therefore, the gamma-ray intensities in the ENDF files are *not* exactly the same as those discussed in the previous section. The normalization factor applied to the data is given on the web site and in the archive for the isotopic data. If the measured energy of the gamma-ray spectrum was greatly different than the available energy, the *un-normalized* data were incorporated into the ENDF evaluations.

A similar format is used for this set of isotopic and elemental data on the web site and archived on HPSS. Examples are given in Appendices E and F for the isotopic and elemental data respectively. As shown in Appendix E, the normalization factor applied to the ^{9}Be gamma-ray intensities was 0.9981. Only gamma-rays with intensities greater than 0.01 times the most intense gamma ray for a given element are listed in the elemental data files. For the sulfur example in Appendix F, there were 29 gamma rays with an intensity greater than 0.6464 per 100 captures. These 29 gamma-rays account for 94.6% of the available energy. The report LA-13812[10] describes the normalization process and creation of the elemental data in detail. *As these data were generated at a different time than the data for the ADNDT paper, differences exist between the two sets of information.*

An HPSS subdirectory *evals* contains the modified ENDF evaluations that were accepted by the National Nuclear Data Center. Additionally, relevant reports are included in PDF format. A listing of the *endf* directories is given below.

```
/hpss/nucldata/mc/special/acti/data/endf

la-ur-98-551.pdf cr52             la13812.pdf       sc45
la-ur-98-543.pdf cr53             li6               si28
la-ur-98-550.pdf cr54             li7               si29
la-ur-98-552.pdf crnat            mg24              si30
la-ur-98-867.pdf cu63             mg25              sinat
al27             cu65             mg26              sm149
al27_d           cunat            mgnat             snat
ar36             f19              mn55              ta181
ar40             fe54             n14               ti46
b10              fe56             na23              ti47
be9              fe57             ne20              ti48
c12              fe58             ne21              ti49
c13              fenat            ne22              ti50
ca40             gd155            ni58              tinat
ca42             gd157            ni60              v51
ca43             ge70             ni61              w182
ca44             ge72             ni62              w183
ca46             ge73             ni64              w184
ca48             ge74             ninat             w186
canat            ge76             o16               zn64
cl35             h1               p31               zn66
cl37             k39              s32               zn67
clnat            k40              s33               zn68
co59             k41              s34
cr50             knat             s36

/hpss/nucldata/mc/special/acti/data/endf/evals

al27.d      cr53.d      fe57.d      mn55.d      ni64.d      w182.d
be9.f       cr54.f      fe58.f      n14.f       o16la.p6    w183.d
```

```
canat.b    cu63.d    h1            na23.f    s32.b     w184.d
cl35la8    cu65.d    he4           ni58.d    sc45.f    w186.d
cl37la8    f19.x     knat.h        ni60.d    snat.b    readme
cr50.f     fe54.f    la13812.pdf   ni61.f    tinat.b
cr52.d     fe56.d    mgnat.f       ni62.f    vnat.b
```

References

1 J. G. Conaway and S. C. Frankle, “Summary Report for Fiscal Year 1993, TTP # AL131004: Multi-Spectral Nuclear Logging,” Los Alamos National Laboratory release, LA-UR-93-4538 (1993).

2 J. G. Conaway et al., “Detection of Contaminants Along Boreholes with Prompt Gamma Spectroscopy,” invited presentation to Annual Meeting of the American Nuclear Society, LA-UR-95-107 (1995).

3 S. C. Frankle, “Photon Production Assessment for the MCNP Data Libraries,” Los Alamos National Laboratory report, LA-13092 (1996).

4 S. C. Frankle and J. G. Conaway, “MCNP Simulations for Identifying Environmental Contaminants Using Prompt Gamma Rays from Thermal Neutron Capture Reactions,” Appl. Radiat. Isot. **48**, 1337-1341 (1997).

5 R. C. Reedy and S. C. Frankle, “Neutron-Capture Yields for Gamma-Ray Spectroscopy,” and S. C. Frankle and P. G. Young, “Improved Photon-Production Data for Thermal-Neutron Capture in ENDF,” Capture Gamma-Ray Spectroscopy and Related Topics: 10th International Symposium, AIP Conf. Proc. 529, 697-702 (2000).

6 Joint Work Statement No. LA95J10236-A001, CRADA No. LA95C10236-A001, Computer Simulation in Support of Nuclear Well-Logging (1995).

7 J. F. Briesmeister, ed., “MCNP - A General Monte Carlo N-Particle Transport Code, Version 4C,” Los Alamos National Laboratory report LA-13709-M (2000).

8 R. C. Reedy and S. C. Frankle, "Prompt Gamma Rays from the Capture of Thermal Neutrons by Elements from Hydrogen through Zinc," accepted by Atomic Data and Nuclear Data Tables (February 2001).

9 V. McLane, C. L. Dunford, and F. Rose, ed., "ENDF-102: Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," Brookhaven National Laboratory report, BNL-NCS-44945 (1997).

10 S. C. Frankle, R. C. Reedy and P. G. Young, "Improved Photon-Production Data for Thermal Neutron Capture in the ENDF/B-VI Evaluations," Los Alamos National Laboratory report, LA-13812 (2001).

Appendix A

Description of Tables for the Isotopic Data

Description of archived isotopic data

TABLE 1 Adopted Prompt Gamma Rays

This entry summarizes the energies and intensities for the prompt gamma rays adopted for the radiative capture of thermal neutrons by this isotope. 'Adopted' in this context means the final gamma-ray energies and intensities assigned to an isotope based on an evaluation of the published data. It also gives a few quantities that summarize the results. The gamma-ray energies (Eg) are in keV. The gamma-ray intensities (Ig) are per 100 neutron captures (or %). Sn is the neutron binding energy (in keV) for the product nucleus.

The first line is a short title. Then comes the number of adopted gamma rays and several sums involving Eg, Ig, or their product. The sum of Eg*Ig is divided by Sn to see if all of the energy available in the reaction is accounted for in the adopted data. The sums of the gamma rays known to have been emitted from the capture state or known to have decayed to the ground state are also given and should be 100% if the data set is complete and if there are few internal conversion electrons.

The adopted gamma-ray results are listed with one gamma ray per line. In addition to the gamma ray's energy and intensity, the energies of the upper and lower levels (if known) for that gamma-ray transition are also given.

TABLE 2 Comments on Adopted Data

This text describes the data sets adopted and gives additional comments on the data for the neutron-capture reaction with this isotope. Complete references are given below under REFERENCES. Often a comment is given on the quality of the adopted energies and intensities.

TABLE 3 Comparisons of Prompt Gamma-Ray Energies and Intensities

After a one-line title, there first is a quick summary of the input data for the product nucleus with the neutron binding energy (Sn), the mass (in amu) of the product nucleus used to get the recoil energy, and the energy levels (keV) in the product nucleus. The number of data sets entered and compared is given followed by the code for each of these data sets in the "Nuclear Science References" (NSR) format (e.g., 96Be53). Complete references are given at the end under REFERENCES.

The set (or sets) of data adopted for the energies and for the intensities of the gamma rays are then given. Adopted sets are identified by their order (1 through 5) and their NSR code. If more than one set is adopted, there is a weighting factor for each set. (Note that if one set is weighted more than another set, then a small fraction of the less weighted set will be averaged, with the lower weight, to get the final adopted value.) Data set 6 always refers to the set of gamma rays whose energies have been calculated by subtracting the recoil energy from the difference in the level energies for the transition. The number of gamma rays from the adopted data with non-zero values of Eg and Ig are given along with the number of entered gamma rays not adopted.

The next part compares, for each gamma ray, the adopted energy (Eg-ad) with the energy calculated from levels (if known) minus the recoil energy (DLv-Er) or with the energy that was entered for each data set. (Note that the energies for some data sets include the recoil energy. This recoil energy has been subtracted to get the energy of the gamma ray.) The recoil energy (Er) is given for each gamma ray. Individual data entries can be flagged (*) such that they are ignored in these comparisons. At the end of the gamma-ray-energy comparison, the number of gamma rays compared and a weighted (by the square root of the adopted intensity Ig) average absolute deviation in energy ("WTD[SQRT(Ig)] AVG [ABS(DELTA-E)]") is given for "DLv-Er" and for each data set. Each value for a given set of energies Eg relative to the adopted energy Eg-ad is

WEIGHTED ABS(DELTA-E) = SUM[SQRT(Ig)*ABS(Eg-ad - Eg)]/Sum[SQRT(Ig)]

where SQRT is square root and ABS is the absolute value.

For intensities, the percent deviation of the input intensity (after any normalization factor, Ig Norm, has been applied) from the adopted ("Ig-ad") intensity are given for each gamma ray. Data entries can be flagged (*) such that they are ignored in these comparisons. At the end of the intensity comparison, the number of gamma rays compared and a weighted (by square root of the intensity Ig) average for these percent deviations is given for each data set:

WEIGHTED AVG[% DEVIATION]=SUM[SQRT(Ig)*ABS(1.0 - (Ig/Ig-ad))]*100/SUM[SQRT(Ig)]

where SQRT is square root and ABS is the absolute value.

A few comparisons are then made for the adopted intensities and for the intensities for each data set. The sum of Eg*Ig and the sum of Eg*Ig divided by Sn are given for each data set. The intensity sum out of the capture level and the intensity sum into the ground state are also given.

Statistics for each of the major levels is then given. A level is considered a major level when one of the sums of the intensity into or out of the level is greater than 0.5%. The number and intensities of gamma rays into and out of the major levels are given. These intensity sums are rounded to the nearest %. (A good set should have about the same "in" and "out" values for every level except the capture state and the ground state.)

TABLE 4 Experimental Prompt Gamma-Ray Data

This table has the published experimental data for gamma-ray energies and intensities used to obtain the adopted gamma rays and to compare data sets. After a title line, there is a line with the name(s) for the entered data set(s). The NSR codes (e.g., 71Ar39) are used and are the same as in the REFERENCES below. Occasionally the data were copied directly from the National Nuclear Data Center (NNDC) website, and those data are often denoted NNDC. Similarly, data copied from the evaluations done by X Division at LANL are denoted as XCI. In a few cases, separate entries are made for different tables in one reference, especially if each table needs to have a different normalization factor.

The next line has the normalization factors applied to the intensities for each data set. Often this normalization factor is just 1.0. In some cases, the data were taken from a website with the strongest gamma ray given an intensity of 100 (as for NNDC) or normalized in some fashion (as for XCI), and the normalization factor converts those intensities to absolute values. A minus sign before the normalization factor indicates that the set's energies include the recoil energy so that the code can convert those energies to gamma-ray energies.

There is one line of information for each gamma ray. After the energies of the levels (rounded to the nearest keV) for the gamma-ray transition (if known) are the energies (in keV) and intensities (nominally in %) for each data set for a given gamma ray. A minus sign before an energy or intensity indicates that that value is ignored in the comparisons.

TABLE 5 Energy Levels for Product Nucleus

The known energy levels for the product nucleus up to and including the capture state are given in keV. After a title line and column headings, there is a line that ends with a number that indicates the approximate value for the largest uncertainty of the level energies in keV.

The energy level data are then given with one level per line. The level's energy in keV is given, and if known, that level's spin (J) and parity are given. A ? indicates that there is some uncertainty in the adopted spin. If there are two possible adjacent spins, such as 1 and 2, then the average of those two values (1.5) is given for the spin and the ? indicates that the spin is not exact. In some cases, 3 adjacent spins are possible (e.g., 1/2, 3/2, and 5/2) and the average (1.5) with a ? indicates that there is an uncertainty in that adopted spin value. The letter C indicates the capture state.

Often the data for these levels were taken from the 8th Edition of the Table of Isotopes (Firestone et al., 1996). That source is often referred to as ToI8 or a similar abbreviation.

REFERENCES

The full references of the literature sources used for that isotope are given here. The references are in the NSR format as taken from the NSR section of the website for the National Nuclear Data Center at the Brookhaven National Laboratory. The NSR format (e.g., 71Ar39 or 1971Ar39) has the year as the first 2 or 4 numbers, then the first 2 letters of the first author's last name, and either a 2 digit number (starting with 01 for journals) or 2 letters (starting with ZZ for other documents). References here are first sorted by year than by the first author's name. In a very few cases, an adopted reference is not in the NSR system and there is nothing after the first two letters of the first author's last name (e.g., 1993Pr).

Appendix B

Example of an Isotopic Data Archive for ^{12}C

12C(n,g)13C

TABLE 1 Adopted Prompt Gamma Rays

Gamma rays from capture of thermal neutrons by 12C   R. Reedy   10/28/99
6 good energy-intensity pairs   SUM Intensities =   132.80 %
Sn= 4946.31 keV   Sum(Eg*Ig)= 494747.9 keV*%   Sum(Eg*Ig)/Sn= 100.02 %
Sum Ig from capture state = 99.99 %   Sum Ig into ground state = 100.04 %

Eg(keV)	Ig/100*n-cap	Up-lvl	Lo-lvl(keV)
595.05	0.240	3684.51	3089.44
1261.74	32.360	4946.31	3684.51
1856.72	0.160	4946.31	3089.44
3089.05	0.430	3089.44	0.00
3683.95	32.140	3684.51	0.00
4945.30	67.470	4946.31	0.00

TABLE 2 Comments on Adopted Data

The intensities of the gamma rays for the capture of thermal neutrons by 12C are those of Mughabghab et al. (1982) [1982Mu14]. The intensities of the three major gamma-ray lines are consistent with those of Thomas et al. (1967) [1967Th05], Rasmussen et al. (1969) [1969Ra10], and Jurney et al. (1982) [1982Ju01]. These intensities differ by only a few percent.

The gamma-ray energies were calculated from the energies of the levels and capture state as reported by Ajzenberg-Selove (1991) [1991Aj01]. The energies of these levels are known to ~0.1 keV. The data appear complete and very good.

TABLE 3 Comparisons of Prompt Gamma-Ray Energies and Intensities

Gamma rays from capture of thermal neutrons by 12C   R. Reedy   10/28/99
NEUTRON BINDING ENERGY =   4946.31 keV   MASS OF A+1 NUCL = 13.0000 AMU

Levels in 13C known to <2 keV (from ToI8, 1996)
5 LEVEL ENERGIES (keV):
0.00 3089.44 3684.51 3853.81 4946.31

6 GAMMA RAYS ENTERED 5 SETS 82Mu14   67Th05   90Wa22   69Ra10   82Ju01

ADOPTED SET 6 (DLv-Er) FOR ENERGY

ADOPTED SET 1 (82Mu14) FOR INTENSITY

6 GAMMA RAYS ADOPTED,   0 GAMMA RAYS NOT ADOPTED

LEVEL ENERGIES, E-RECOIL (Er), ADOPTED ENERGIES (Eg-ad), AND DELTA E
(all in keV) FOR 5 SETS   (-- = NOT 2 VALUES TO COMPARE)   (* = IGNORED)

NUMBER OF GAMMA RAYS ENTERED =						6	3	1	3	2
					Eg-ad MINUS DLv-Er OR entered Egs					
Gam#	Level Energies		Er	Eg-ad	DLv-Er	82Mu14	67Th05	90Wa22	69Ra10	82Ju01
1	3684.51	3089.44	0.01	595.05	0.00	-0.45	--	--	--	--
2	4946.31	3684.51	0.07	1261.74	0.00	0.14	-0.26	--	0.54	--
3	4946.31	3089.44	0.14	1856.72	0.00	0.12	--	--	--	--
4	3089.44	0.00	0.39	3089.05	0.00	-0.45	--	--	--	--
5	3684.51	0.00	0.56	3683.95	0.00	-0.05	-0.05	0.03	0.05	-0.05
6	4946.31	0.00	1.01	4945.30	0.00	-0.02	0.30	--	0.10	-0.70
# Eg in weighted average =					6	6	3	1	3	2
WTD[SQRT(Ig)] AVG [ABS(DELTA-E)]=					0.00	0.09	0.22	0.03	0.21	0.44

PERCENT DEVIATIONS OF INTENSITIES RELATIVE TO ADOPTED SET
(* = IGNORED) (-- = NOT 2 VALUES TO COMPARE)

Gam#	Eg-ad	Ig-ad	82Mu14	67Th05	90Wa22	69Ra10	82Ju01
		Ig Norm =	1.0000	1.0000	1.0000	1.0040	1.0000
1	595.05	0.240	0.0	--	--	--	--
2	1261.74	32.360	0.0	5.1	--	9.4	--
3	1856.72	0.160	0.0	--	--	--	--
4	3089.05	0.430	0.0	--	--	--	--
5	3683.95	32.140	0.0	5.8	--	0.7	3.5
6	4945.30	67.470	0.0	2.2	--	0.3	1.7
# Ig in wtd average =			6	3	0	3	2
WTD AVG [% DEVIATION]=			0.0	4.1	0.0	3.1	2.4
SUM Ig =		132.800	132.800	134.000	0.000	128.512	99.600

NEUTRON BINDING ENERGY (Sn) = 4946.31 keV

	Adopted	82Mu14	67Th05	90Wa22	69Ra10	82Ju01
SUM (Eg*Ig)	494747.9	494746.8	494621.9	0.0	487332.4	453586.3
SUM(Eg*Ig)/Sn	100.02	100.02	100.00	0.00	98.52	91.70
SUM FROM CAP LVL	99.990	99.990	100.000	0.000	96.585	68.600
SUM INTO GRD LVL	100.040	100.040	100.000	0.000	99.195	99.600

IN-OUT STATISTICS FOR MAJOR LEVELS

		NUMBERS		INTENSITY (IN - OUT) IN %					
Lvl	E-lvl	In	Out	Adopted	82Mu14	67Th05	90Wa22	69Ra10	82Ju01
1	0.0	3	0	100.- 0.	100.- 0.	100.- 0.	0.- 0.	99.- 0.	100.- 0.
3	3684.5	1	2	32.- 32.	32.- 32.	34.- 34.	0.- 0.	29.- 32.	0.- 31.
5	4946.3	0	3	0.-100.	0.-100.	0.-100.	0.- 0.	0.- 97.	0.- 69.

TABLE 4 Experimental Prompt Gamma-Ray Data

Gamma rays from capture of thermal neutrons by 12C R. Reedy 10/28/99

		82Mu14		67Th05		90Wa22		69Ra10		82Ju01	
		1.0000		1.00		1.0		1.004		1.00	
3685	3089	595.5	0.24								
4946	3685	1261.6	32.36	1262.	34.			1261.2	29.2		
4946	3089	1856.6	0.16								
3089	0	3089.5	0.43								
3685	0	3684.0	32.14	3684.	34.	3683.915		3683.9	31.8	3684.	31.0
4946	0	4945.32	67.47	4945.	66.			4945.2	67.0	4946.	68.6

TABLE 5 Energy Levels for Product Nucleus

Levels in 13C known to <2 keV (from ToI8, 1996)

E(keV)	J	2.0
0.0	0.5-	
3089.443	0.5+	
3684.507	1.5-	
3853.807	2.5+	
4946.31	0.5+C	

REFERENCES

1967Th05 G.E.Thomas, D.E.Blatchley, L.M.Bollinger
High-Sensitivity Neutron-Capture Gamma-Ray Facility
Nucl.Instr.Methods 56, 325-337 (1967)

1969Ra10 N.C.Rasmussen, Y.Hukai, T.Inouye, V.J.Orphan
Thermal Neutron Capture Gamma-Ray Spectra of the Elements
AFCRL-69-0071 (MITNE-85) (1969)

1982Ju01 E.T.Jurney, P.J.Bendt, J.C.Browne
Thermal Neutron Capture Cross Section of Deuterium
Phys.Rev. C25, 2810-2811 (1982)

1982Mu14 S.F.Mughabghab, M.A.Lone, B.C.Robertson
Quantitative Test of the Lane-Lynn Theory of Direct Radiative Capture of Thermal Neutrons by 12C and 13C

Phys.Rev. C26, 2698-2701 (1982)

1990Wa22 A.H.Wapstra
Energy Calibration for 2-13 MeV Gamma Rays
Nucl.Instrum.Methods Phys.Res. A292, 671-676 (1990)

1991Aj01 F.Ajzenberg-Selove
Energy Levels of Light Nuclei A=13-15
Nucl.Phys. A523, 1-196 (1991)

Appendix C

Description of Tables for the Elemental Data

Description of archived elemental data

TABLE 1 Prompt Elemental Neutron-Capture Gamma Rays Sorted by Intensity

The prompt gamma rays from radiative capture of thermal neutrons adopted for this element are listed after being sorted by decreasing intensity. The gamma-ray energies (Eg) are in keV. The gamma-ray intensities (Ig) are per 100 neutron captures (or %) for that element. The isotope that captured the thermal neutron (i.e., the target nucleus) to make that gamma ray is given in the last column. Only gamma rays above a specified intensity threshold (given in Table 3) are listed.

TABLE 2 Prompt Elemental Neutron-Capture Gamma Rays Sorted by Energy

The adopted prompt gamma rays from radiative capture of thermal neutrons for this element are sorted in order of increasing energy. The gamma-ray intensities (Ig) are per 100 neutron captures (or %) for that element. The third column contains rounded-off values of the intensities from this work as reported in Atomic Data and Nuclear Data Tables (ADNDT) for elements from H through Zn (Z = 1 - 30). For intensities greater than 30%, the values in the ADNDT article were later modified to include one digit after the decimal point. The isotope that captured the thermal neutron (i.e., the target nucleus) to make that gamma ray is given in the last column. Only gamma rays above a specified intensity threshold (given in Table 3) are listed.

TABLE 3 Summaries and Data Used to Convert Isotopic Data to Elemental Data

The seven subtables of Table 3 give the data used to convert the isotopic data for capture gamma rays to elemental data. They also provide summary information for the prompt isotopic and elemental capture gamma-ray data.

The first subtable lists the data used to calculate the fraction of neutron captures by each isotope ("Reac Frac") for an element. The key data for this calculation are the atom fraction of an isotope ("Atom-frac") and that isotope's cross section in barns for radiative capture at thermal neutron energies ("XS(b)"). The isotopic fractions are the “representative isotopic compositions” of Table 1 from Rosman and Taylor, J. Phys. Chem. Ref. Data vol. 27, pp. 1275-1287 (1998). The thermal cross sections are from Holden, "CRC Handbookof Chemistry and Physics," Section 11 (1999). The "Reac Frac" is the atomic fraction and cross section weighted contribution at thermal neutron energies.

Reac Frac(iso) = [XS(iso)*Atom-frac(iso)]/[SUM(XS(iso)*Atom-frac(iso))]

The last two lines of the subtable give the calculated ("Totals") and measured ("Nat-elem") elemental atomic weights and capture cross sections (as a check of the calculations) and determines the average amount of energy produced per elemental capture (Sn, in keV). The elemental average energy is

Sn(element) = SUM (Reac-Frac(iso) * Sn(iso))

The second subtable gives summary information for the isotopic data. For each isotope, Ng is the number of adopted gamma rays, S(Ig) is the sum of isotopic intensities (in %), Sn is the neutron binding energy (in keV), S(E*I)/Sn is the sum of Eg*Ig divided by Sn (in %), and S(cap) and S(grd) are the sums (in %) of intensities of gamma rays from the capture state and into the ground state. The quantity S(E*I)/Sn should be equal to 100.0% if all of the capture gamma-rays have been measured. Additionally, if all the gamma-rays out of the capture state or into the ground state have been measured, S(cap) and S(grd) should be 100.0.

The third subtable gives, for each isotope, the number of gamma rays for various intensity bins of Ig (10-100%, 1-10%, 0.1-1%, 0.01-0.1%, and <0.01%). The number in each bin indicates the number of gamma rays that have an Ig value greater or equal to the lowest bound for that bin and less than the lower bound for the previous column. The upper bound for the first bin is 100%. Also given are the largest (I-max) and smallest (I-min) of the adopted intensities (Ig).

The fourth subtable lists the maximum ("Imax") and minimum ("Imin") isotopic ("-iso") intensities and elemental ("-el") intensities using the reaction fractions calculated in the first subtable. The last two lines give the largest value of Imin for that element (Imin-el) and the lowest value of elemental intensity saved. If there are not many gamma rays, the lowest value of the elemental intensity saved is often equal to the largest Imin-el. If there are many gamma rays, a higher value is used so as not to list a huge number of elemental gamma rays.

The fifth subtable gives the number and range of elemental intensities of gamma rays saved for each isotope.

The sixth subtable summarizes the data saved for this element. Ng is the number of gamma rays, S(Ig) is the sum of the intensities adopted for this element in Tables 1 and 2 (in %), Sn is the elemental binding energy (in keV), and S(E*I)/Sn (in %) is the sum of Eg*Ig divided by Sn. The table also lists (in %) the largest (I-max) and smallest (I-min) of the adopted elemental intensities. Note that this summary information only includes the gamma rays listed in the tables and therefore often does not include the weakest gamma rays for a specific element.

The last subtable gives the number of elemental gamma rays in various intensity bins (30-100%, 10-30%, ... , 0.03-0.10%, 0.01.-0.03%, and <0.01%). Each bin gives the number of gamma rays with Ig values greater to or equal to the lowest bound for that bin and less than the lower bound for the previous column. The upper bound for the first bin is 100%.

Appendix D

Example of an Elemental Data Archive for C

Data for 10 Prompt Gamma Rays Made by the Capture of Thermal Neutrons
by 2 Isotopes of Z = 6 Carbon (C) Cross section = 3.50E-03 b

TABLE 1 Prompt Elemental Neutron-Capture Gamma Rays Sorted by Intensity

#	Eg (keV)	Ig (#/100)	Isot
1	4945.30	67.179	12C
2	1261.74	32.221	12C
3	3683.95	32.002	12C
4	3089.05	0.428	12C
5	8173.92	0.362	13C
6	595.05	0.239	12C
7	1856.72	0.159	12C
8	6092.40	0.070	13C
9	1586.80	0.037	13C
10	495.40	0.034	13C

TABLE 2 Prompt Elemental Neutron-Capture Gamma Rays Sorted by Energy

Eg (keV)	Ig (#/100)	Ig-ADNDT (#/100)	Isot
495.4	0.034	0.03	13C
595.0	0.239	0.24	12C
1261.7	32.221	32.	12C
1586.8	0.037	0.04	13C
1856.7	0.159	0.16	12C
3089.1	0.428	0.43	12C
3683.9	32.002	32.	12C
4945.3	67.179	67.	12C
6092.4	0.070	0.07	13C
8173.9	0.362	0.36	13C

TABLE 3 Summaries and Data Used to Convert Isotopic Data to Elemental Data

2 Isotopes Z = 6 Carbon (C)

A	Atom-frac	At-Wt	Sn(keV)	XS(b)	Reac Frac
12	0.989300	12.00000	4946.31	0.003500	0.99569
13	0.010700	13.00336	8176.44	0.001400	0.00431
Totals	1.000000	12.01074	4960.22	0.003478	1.00000
	Nat-Elem	12.01070		0.003500	

Isot	Ng	S=Sum S(Ig)	E-keV Sn-keV	Intensities-% S(E*I)/Sn	S(cap)	S(grd)
12C	6	132.8	4946.31	100.0	100.0	100.0
13C	7	127.8	8176.44	100.0	99.9	100.3

- - - - - - % Intensities (Isotopic) - - - - - -

Isot	Ng	>10	1-10	.1-1	.01-.1	<.01	I-max	I-min
12C	6	3	0	3	0	0	67.5	0.160
13C	7	2	5	0	0	0	84.0	2.500

Maximum & Minimum Elemental Intensity Fractions for Isotopes

Isot	Reac Frac	Imax-iso	Imax-el	Imin-iso	Imin-el
12C	0.99569	67.470	67.179	0.1600	0.1593
13C	0.00431	84.000	0.362	2.5000	0.0108

Largest Imin-el is 0.1593 For A = 12
Lowest elemental intensity saved = 0.030 %

Elemental intensities 10 Gamma rays for Z = 6 (C)

Isot	N-gam	Largest-I	Smallest-I
12C	6	67.179	0.159
13C	4	0.362	0.034

		S=Sum	E-keV	Intensities-%		
Z	Ng	S(Ig)	Sn-keV	S(E*I)/Sn	I-max	I-min
6 C	10	132.7	4960.2	100.0	67.2	0.0345

		- - - - - - % Intensities (Elemental) - - - - - - -								
		30	10	3	1	.3	.1	.03	.01	
Z	Ng	-100	-30	-10	-3	-1	-.3	-.1	-.03	<.01
6 C	10	3	0	0	0	2	2	3	0	0

Appendix E

Example of an Isotopic Data File for ENDF Modifications of ^{9}Be

```
Recommended thermal neutron capture spectrum for Be-9.
Yield was normalized to a Q-value of 6.81238 MeV.
Normalization factor = 0.9981.



Number of gamma-rays
11

Egamma    Igamma
(keV)  #/100 captures
219.3    4.991E-02
547.4    1.597E-01
631.8    2.395E-01
853.6    2.346E+01
2590.0    2.256E+01
2811.8    1.298E-01
2896.4    1.497E-01
3367.6    3.304E+01
3443.6    1.058E+01
5956.6    1.487E+00
6809.9    6.538E+01
```

Appendix F

Example of an Elemental Data File for ENDF Modifications of S

```
Top 29 Gamma-rays for Natural S from thermal neutron capture
normalized to the (cross-section*atomic fraction) weighted Q-value.
These gamma-rays account for 94.6 % of the available energy.

Q-value    8.60238

Number of gamma-rays
    29

Egamma     Igamma
keV    #/100 captures
841.0    64.6462
1225.7    0.6369
1472.4    1.7243
1572.3    0.8545
1697.3    2.5292
1964.8    1.3301
1967.1    0.7680
2216.7    2.4923
2313.4    0.7311
2347.7    1.2278
2379.7    43.0975
2490.2    2.5292
2667.7    0.7117
2753.3    5.3777
2867.5    0.8990
2930.7    16.3021
3220.6    23.2352
3369.8    5.0030
3397.5    1.0495
3723.7    2.5292
4430.8    4.7224
4637.9    1.3522
4869.6    12.1797
5047.1    3.0360
5420.6    56.5889
5583.7    1.4049
5888.1    0.7117
7799.8    2.5670
8640.5    1.7243
```

Distribution:
X-5 files

Campbell, J. M.	X-5	MS F663
Comly, J. C.	X-5	MS F663
Court, D.	X-5	MS F663
Estes Guy P.	X-5	MS F663
Favorite, J.	X-5	MS F663
Forster, R. A.	X-5	MS F663
Frankle Stephanie C.	X-5	MS F663 (2 copies)
Heath, Alexandra R.	X-5	MS F663
Little, Robert C.	X-5	MS F663
Roberts, Roger	X-5	MS F663
Seed, Thomas	X-5	MS F663
Sood, Avneet	X-5	MS F663
White, M.	X-5	MS F663
Young, P. G.	T-16	MS B243
Reedy, R.	NIS-2	MS D436

Web distribution