Chapter 5: Binary Data File Formats

Overview

TART95 uses four binary data files. The default names and contents of these data files are,

1) TARTND - Neutron Interaction data
2) TARTPPD - Neutron induced photon production data
3) GAMDAT - Photon interaction data
4) NEWCROSS - Multiband parameters

In principle the formats for these files are quite general. In practice the files have been very stable and have changed very little over the last few years. Below both general parameters and their current values are described.

Below each file will be described by defining what is stored in each word of the file, from start to end. In addition it will be indicated when certain words that are actually stored later in the file must be read earlier in order to allow data stored earlier in the file to be correctly interpreted.

Data File Use

The TART95 binary data files are designed to be used on virtually any computer. The processed data files are written in character form that can easily be copied to any computer, where they are then converted to binary, random access form, compatible for use on that computer. On any computer the files are created and accessed using standard FORTRAN binary, random access statements that work on any computer. This operation has now been successfully performed on every computer from an IBM-PC to a CRAY super computer. As such, it is not accurate to say that the files are binary compatible between computers, e.g., the files prepared for use on a SUN workstation cannot be used on an SGI workstation. However, what is important is that these binary, random access files can be accurately implemented and used on virtually any computer.

In order to develop data files that can be used on virtually any computer the format and layout of the TART95 data files differ slightly from those used by the production version of TART, which is only designed to operate on a CRAY computer. The files used by the production version of TART rely on the CRAY 64 bit per word structure and pack words. In contrast the TART95 files can be correctly used on 32 or 64 bit per word computers and do not contain any packed words; each piece of information is assigned its own unique word in the TART95 data files. **WARNING** - the TART95 data files described here are not compatible for use with the CRAY production version of TART, neither is the layout of each file described here identical to the layout of the CRAY production data files. For a comparison of the two see the earlier documentation of TART.

All of the TART95 binary data files are in standard FORTRAN binary, random access format. The files are written in fixed length records of 10,000 words each. TART95 uses simple FORTRAN routines to open and access the files as if they were a continuous string of words starting from address zero (0), not one (1), and proceeding sequentially. The simple FORTRAN routines handle all of the logic involved in mapping the fixed length records to make them look to TART95 like a continuous string of words, i.e., TART95 need not know anything about the fixed length records.

The files are written in single precision, e.g., 32 bits per word on a SUN workstation and 64 bits per word on a CRAY. The files contain a mixture of floating and fixed point variables as well as character strings. By using the convention to only store up to four characters per word in character arrays, using single precision completely eliminates all potential conflicts in mixing together floating, fixed and character words.

Since TART95 uses multigroup data, single precision is more than adequate to represent all of the data to well beyond the accuracy to which it is known.

Data File addresses

In the data files the address is defined sequentially starting from zero (0), not one (1).

Characters from Data Files

Each data file has a string of characters near its beginning to identify the file. It also has strings of characters to identify the date of each evaluation. TART95 reads two words in 2A4 format to define the library date, in the form MM/DD/YY, e.g., 6/21/92, stored four characters in each word. It also reads one word per evaluation in A4 format to define the date of the evaluation, in the form, YYMM, e.g., 9206. These are the only characters read from the data files.

Data File Sizes

The binary, random access files used by TART95 are quite small, so that they can be easily implemented on virtually any computer,

	Words	Fixed Length Records (10,000 words each)
TARTND	500,000	50
TARTPPD	330,000	33
GAMDAT	140,000	14
NEWCROSS	170,000	17
Total	1,140,000	114

Regardless of how much data is actually read from the files the use of fixed length records for binary, random access, means there are never very many actual reads from the files,

e.g., if every single evaluation in TARTND were used it would only require 50 actual reads from the file.

Data File Contents

In the following description of the data files the contents of each word will be described starting from address zero (0) and working sequentially upwards. The numbers over the descriptions define the address of each word in the file.

In principle the format of the neutron interaction data file (TARTND) and the neutron induced photon production data file (TARTPPD) are identical. They are identical as far as the header information at the beginning of each file (the first 3813 words), but differ in the actual contents of the data defined for each evaluation.

TARTND and TARTPPD: Common Header Information

0
Not used

1
Number of evaluations (150). Note, this word specifies 150 in order to allocate storage for up to this many evaluations. Currently only 110 evaluations are included and the remainder of the table is zero.

2 - 601
The evaluation map. Four words are specified for each evaluation,

1 - ZA
2 - First word address
3 - Total size of evaluation in words
4 - Atomic Weight

The data is stored as 150 values ZA, followed by 150 first word addresses, followed by 150 sizes, followed by 150 atomic weights = 600 words. In each case only 110 values are used and the remainder of each array is zero.

Note, in order to correctly interpret the following data, words 3809-3813, described below, must be read before the following data.

602-777 (176 values)
Speed, in cm/shake, corresponding to multigroup boundaries.

778-953 (176 values)
Multigroup boundaries, in MeV.

954-3808 (2855 words)
Five tables, each 571 words long, used for multigroup indexing.

In general the following five (5) words are stored in the five words immediately preceding the start of the first evaluation. Their location is defined from the evaluation map as five (5) words less than the starting address of the first evaluation.

3809-3810
Library date, in the form MM/DD/YY, e.g., 6/21/92, stored four characters in each word.

3811
Number of multigroup boundaries (176 = one more than the number of multigroups). This must be read earlier to define the number of multigroup boundaries to read from addresses 602-777 and 778-953,

3812
Size of arrays used for multigroup indexing (571). This must be read earlier to define of the size of the five tables in addresses 954-3808.

3813
Number of equally probable bins in angular distributions (32)

3814
Start of first evaluation. From this point on the layout of the file depends on the details of each evaluation.

The order of evaluations is from lowest ZA to highest ZA, starting with the neutron, ZA = 1, up to ZA = 98252, the highest real ZA, and finally ending with the ENDL convention that Z = 99 means fission products.

The data for each evaluation starts with,

1 - Total size of evaluation in words
2 - Date of evaluation
3 - ZA
4 - Atomic Number Z (floating point)
5 - Atomic weight
6 - Number of kinematics type lists
7 - Number of reactions

The following are repeated for each kinematics type list,

(words = number of reactions)
Number of words after the last energy deposit list to complete the description of each reaction.

(words = number of reactions)
Kinematics type for each reaction.

(words = 2 x number of reactions)
Minimum followed by maximum multigroup index for each reaction.

(words = 4 x number of reactions)
Q value and C, I, S for each reaction.

The data for each reaction follows,

1 - The number of different types of energy deposition.

(words = maximum - minimum multigroup indices + 1)
Cross section for the reaction. Note, cross sections and energy deposition for each reaction are defined starting at the defined minimum group index and ending at the maximum group index = (maximum - minimum + 1) words.

(words = maximum - minimum multigroup indices + 1)
Energy deposition for the reaction. This is repeated based on the number of different types of energy deposition, defined above. There may be zero (0) or more types of energy deposition.

From this point on the layout depends on the collision type and differs for TARTND and TARTPPD. The format of the data depends on the collision type, or kinematics method (the two terms are used interchangeably) . Below is a summary of the collision types and how many times each is used in the current data files (in parenthesis following each collision type).

Neutron Interactions (TARTND)

Only types 1, 2, 3, 4, 5, 9, 12, 14 and 19 are currently used. Most of the other types were used in earlier versions of the data files, but will most probably never be used again.

Types 8 and 15 are used only for n,2n reactions and are controlled by **sentl 50** (see **TART95 Input**). These types use special tabulated, correlated distributions that assume one high and one low energy neutron, correlated in that sampling is symmetric about the midpoint of the distributions. No extra data for these types is included in TARTND. When **sentl 50** is set the existing n,2n distributions in TARTND are divided into low and high energy distributions for correlated sampling.

1 = Anisotropic Elastic Scattering (109)
2 = Absorption (261)
3 = Inelastic scattering, Isotropic in Center of Mass (176)

4 = Inelastic scattering, Anisotropic in Center of Mass (56)
5 = Tabulated; Energy and Angle Correlated in Lab (1)
6 = Combined Anisotropic Wide Level and Tabular
7 =
8 = Tabulated n,2n, Isotropic in Lab
9 = Tabulated, Isotropic in Lab (326)
10 =
11 =
12 = Cluster Model, Isotropic in Center of Mass (1)
13 = Tabulated, Energy and Angle Uncorrelated in Lab
14 = Tabulated, Energy and Angle Uncorrelated in Lab (9)
15 = Tabulated n,2n, Anisotropic in Lab
16 =
17 =
18 =
19 = Tabulated Fission Spectra, Isotropic in Lab (76)
20 =
21 =
22 =
23 =
24 = Tabulated Fission Spectra, Isotropic in Lab

Neutron Induced Photon Production (TARTPPD)

All of the following types are currently used.

103 = Line Source, Isotropic in Laboratory (126)
104 = Line Source, Anisotropic in Laboratory (17)
109 = Tabulated Spectra, Isotropic in Laboratory (262)
115 = Tabulated Spectra, Anisotropic in Laboratory (1)

TARTND: Neutron Interaction Collision Types

Collision type 1 = Anisotropic Elastic Scattering

1 - Number of angular distributions
2 - Number of entries in an anisotropic distribution
3 - Least energy group index for the least anisotropic distribution
4 - = 1 - No longer used as an option

5 - List of energies at which angular distributions are given
6 - Equally probable Cosines from -1 to +1.

Note. for 32 equally probable bins, 33 Cosines are given to define the beginning and end of all Cosine intervals.

Collision type 2 = Absorption

No additional information is needed.

Collision type 3 = Inelastic scattering, Isotropic, in CM

1 - Energy of excited level

Collision type 4 = Inelastic scattering, Anisotropic, in CM

1 - Number of angular distributions
2 - Number of entries in an anisotropic distribution
3 - Energy of excited level

4 - List of energies at which angular distributions are given
5 - Equally probable Cosines from -1 to +1.

Note. for 32 equally probable bins, 33 Cosines are given to define the beginning and end of all Cosine intervals.

Collision type 5 = Tabulated; Energy and Angle Correlated in Lab

1 - Number of Incident energies
2 - Number of Cosines
3 - Not Used
4 - Number of Secondary energies
5 - Not Used

1 - Loop over incident energies
2 - Incident Energy
3 - Equally Probable Cosines
4 - Loop over Equally Probable Cosines
5 - Equally Probable Secondary Energies

Collision type 6 = Anisotropic Wide Level and Tabular

This model is no longer used by TART95.

Collision type 7 = NOT USED

Collision type 8 = Tabulated n,2n, Isotropic in Lab

Types 8 and 15 are used only for n,2n reactions and are controlled by **sentl 50** (see **TART95 Input**). These types use special tabulated, correlated distributions that assume

one high and one low energy neutron, correlated in that sampling is symmetric about the midpoint of the distributions. No extra data for these types is included in TARTND. When **sentl 50** is set the existing n,2n distributions in TARTND are divided into low and high energy distributions for correlated sampling.

Collision type 9 = Tabular, Isotropic in Lab

The number of emitted neutrons is **independent** of energy.

1 - Number of entries in each tabulated spectrum
2 - Number of spectra tables

3 - List of speeds at which spectra are given
4 - Equally probable emission spectra

Collision type 10, 11 = NOT USED

Collision type 12 = Cluster Model, Isotropic in CM

No additional information is needed.

Collision type 13, 14 = Energy and Angle Uncorrelated in Lab

For type 13 the number of neutrons emitted is **dependent** on the neutron energy. For type 14 the number of neutrons emitted is **independent** of the neutron energy.

Only type 14 is used in TART95; not type 13.

It is assumed that the spectra and angular distribution are both given at the same energies.

1 - Number of entries in each tabulated spectrum
2 - Number of spectra tables; assumed to be the same as number of angular distributions
3 - Number of entries in an anisotropic angular distribution
4 - Not used

5 - List of speeds at which spectra are given
6 - Equally probable Cosines from -1 to +1.
7 - Equally probable emission spectra

Note. for 32 equally probable bins, 33 Cosines are given to define the beginning and end of all Cosine intervals.

Collision type 15 = Tabulated n,2n, Anisotropic in Lab

Types 8 and 15 are used only for n,2n reactions and are controlled by **sentl 50** (see **TART95 Input**). These types use special tabulated, correlated distributions that assume one high and one low energy neutron, correlated in that sampling is symmetric about the midpoint of the distributions. No extra data for these types is included in TARTND. When **sentl 50** is set the existing n,2n distributions in TARTND are divided into low and high energy distributions for correlated sampling.

Collision type 16, 17, 18 = NOT USED

Collision type 19 = Fission Spectra, Isotropic in Lab

Both the fission cross section and nu-bar (average number of neutrons emitted per fission) are given as a function of energy. The fission cross section is treated as any other reaction cross section, nu-bar has no energy deposition, but has multiple spectra evaluated as is used in collision type 9 and 10. The number of neutrons emitted is energy **dependent** and is defined by nu-bar. The format is the same as for collision type 9 and 10.

1 - Number of entries in each tabulated spectrum
2 - Number of spectra tables

3 - List of speeds at which spectra are given
4 - Equally probable emission spectra

Collision type 20 , 21, 22, 23 = NOT USED

Collision type 24 = Fission Spectra, Isotropic in Lab

Both the fission cross section and nu-bar (average number of neutrons emitted per fission) are given as a function of energy. The fission cross section is treated as any other reaction cross section, nu-bar has no energy deposition, but has multiple spectra evaluated as is used in collision type 9 and 10. The number of neutrons emitted is energy **dependent** and is sampled from a Poisson distribution that has an average value of nu-bar. The format is the same as for collision type 9 and 10.

1 - Number of entries in each tabulated spectrum
2 - Number of spectra tables

3 - List of speeds at which spectra are given
4 - Equally probable emission spectra

TARTPPD: Neutron Induced Photon Production Collision Types

Collision type 103 = Line Source, Isotropic in Lab

The format is exactly the same as for collision type 3, isotropic inelastic scattering.

1 - Energy of the line

Collision type 104 = Line Source, Anisotropic in Lab

The format is exactly the same as for collision type 4, anisotropic inelastic scattering.

1 - Number of angular distributions
2 - Number of entries in an anisotropic distribution
3 - Energy of the line

4 - List of speeds at which angular distributions are given.
5 - Equally probable Cosines from -1 to +1.

Note. for 32 equally probable bins, 33 Cosines are given to define the beginning and end of all Cosine intervals.

Collision type 109 = Tabulated Spectra, Isotropic in Lab

The format is exactly the same as for collision type 9, tabulated spectra, isotropic in laboratory system.

1 - Number of entries in each tabulated spectrum
2 - Number of spectra tables

3 - List of speeds at which spectra are given
4 - Equally probable emission spectra

Collision type 115 = Tabulated Spectra, Anisotropic in Lab

The format is exactly the same as for collision type 13 or 14, tabulated spectra, anisotropic in laboratory system.

1 - Number of entries in each tabulated spectrum
2 - Number of spectra tables; assumed to be the same as number of angular distributions
3 - Number of entries in an anisotropic angular distribution
4 - Not used

5 - List of speeds at which spectra are given
6 - Equally probable Cosines from -1 to +1.
7 - Equally probable emission spectra

Note. for 32 equally probable bins, 33 Cosines are given to define the beginning and end of all Cosine intervals.

GAMDAT: Photon Interaction Data

0-1
Library date, in the form MM/DD/YY, e.g., 6/21/92, stored four characters in each word.

2
No longer used

3-28
26 words of control information

1 - Size of etab (26)
2 - Size of one ftab table (201); size of ftab is (1)(2)=(26*201 = 5226)
3 - Size of chitab + 1 (501)
4 - Size of gamtab (65)
5 - Size of header for photon cross sections (41 = 13 control + 28 f)
6 - Number of fixed energy points (176)
7 - Number of evaluations in file (99)
8 - Number of isotopes and elements(189)

9 - Starting address of evaluation map (29)
10 - Starting address of ZA of each isotope and element (129)
11 - Starting address of Z of each isotope and element (318)
12 - Starting address of atomic weight of isotope or element (507)
13 - Starting address of internal material numbers (696)
14 - Starting address of ftab (885)
15 - Starting address of chitab (6111)
16 - Starting address of gamtab (6612)
17 - Starting address of etab (6677)
18 - Starting address of ediftb (6703)
17 - Starting address of lltab (6728)
18 - Starting address of fixed energy points (6904)
19 - Starting of data for first evaluation (7080)
20-26 - Not used

29-128 (100 words)
Address of the start of each evaluation

129-317 (189 words)
ZA of each isotope or element

318-506 (189 words)
Z of each isotope or element

507-695 (189 words)
Atomic Weight of each isotope or element

696-884 (189 words)
Internal material number of each isotope or element

885-6110 (5226 words)
26 x 201 ftab = integral of Klein-Nishina at 26 energies; 200 equally probable bins for sampling

6111-6611 (501 words)
chitab = incoherent scattering function data

6612-6676 (65 words)
gamtab = coherent form factor data

6677-6702 (26 words)
etab = energies at which ftab is defined

6703-6727 (25 words)
ediftb = 1/[etab(i) - etab(i-1)]

6728-6903 (176 words)
lltab = relates photon energy to energies at which ftab is given

6904-7079 (176 words)
176 fixed energy points used by all evaluations

7080
Start of data for first evaluation.

The above information is output once at the beginning of the file. The following information is output for Z = 1 through 98, and Z = 99 (fission products); this is output 99 times,

13 - control information

1 - Element number (1 to 99)
2 - Number of energy points (176)
3-13 - Reaction numbers; 11 of them (5,2,1,3,0,0,0,0,0,0,0).
These reaction numbers correspond to,
5 = photoelectric
2 = incoherent
1 = coherent
3 = pair production

28 - f parameters

Most of these 28 parameters are used to define fluorescence emission.

1 - Z (Floating point)
2 - wincoh - 90.368286 $Z^{-2/3}$ - 137 $[2/(3\ mc^2)]^{1/2}\ Z^{-2/3}$
3 - wcoh - 536.358 $Z^{-1/3}$ - 137 $[2/mc^2]\ Z^{-1/3}$
4 - edge(2) - K edge energy
5 - flork - K shell fluorescence yield (for K shell vacancy)
6 - florkl - L shell fluorescence yield (for K shell vacancy)
7 - edge(3) - L_1 edge energy
8 - edge(4) - L_2 edge energy
9 - edge(5) - L_3 edge energy
10 - florl - L shell fluorescence yield (for L shell vacancy)
11 - florm - M shell fluorescence yield (for L shell vacancy)
12 - edge(6) - M_1 edge energy
13 - edge(7) - M_2 edge energy
14 - edge(8) - M_3 edge energy
15 - edge(9) - M_4 edge energy
16 - edge(10) - M_5 edge energy
17 - pka1 - probability of K -> L_3
18 - pka2 - probability of K -> L_2
19 - pkb1 - probability of K -> M_3
20 - pvk - probability of K vacancy (above K edge)
21 - pvkl - probability of L vacancy (above K edge)
22 - pvkm - probability of M vacancy (above K edge)
23 - prestk - probability of Other vacancy (above K edge)
24 - pvl - probability of L vacancy (above L_3, below K)
25 - pv1m - probability of M vacancy (above L_3, below K)
26 - prestl - probability of Other vacancy (above L_3, below K)
27 - probability of L_2 -> M_4 (0.371)
28 - probability of L_3 -> M_5 (0.629)

The 41 words (13 control + 28 f parameters) is followed by,

704 - 176 x 4 cross sections (photoelectric, coherent, incoherent, pair)
528 - 176 x 3 energy deposition (photoelectric, incoherent, pair)

The total size of the data for each evaluation is the same for all evaluations,

13 - control information
28 - f parameters
1273 - cross sections and energy deposition

1314 - Words per evaluation

The total size of the entire file is,

1314 - Words per evaluation
99 - 98 elements plus fission products

130,086 - total words for 99 evaluations
7,080 - words 0 through 7079 at the beginning of the file

137,166 - total words in file
140,000 - rounded up to 10,000 word fixed length records

NEWCROSS: Neutron Cross Section Self-Shielding Data

0 - Number of words in data file I.D. (24)
1 - Starting address of data file I.D. (6)
2 - Number of multigroup boundaries (176)
3 - Starting address of multigroup boundaries (30)
4 - Number of evaluations (110)
5 - Starting address of evaluation map (206)

6-29
Data file I.D. 24 words of text only using four characters (A4 format) per word. Only the first two words are used by TART95, to define the date that the data file was created, in the form MM/DD/YY, e.g., 6/21/92, stored four characters in each word.

30-205
Multigroup boundaries, from lowest energy (1.307E-9 MeV) to highest energy (2.0E+01 MeV). These boundaries are not used by TART95.

206-1205
Five words per evaluation are used in the evaluation map to define each evaluation. This map occupies words 206 through 1205, allowing space for up to 200 evaluations, even though currently only 110 are used; the remainder of the table is zero.

1 - ZA, e.g., oxygen 16 = 8016
2 - Number of cross section bands (2)
3 - Number of words per cross section band (3 through 5)
4 - Starting address, e.g., for the first evaluation 1211.
5 - Temperature in Kelvin (299.0)

Note, the number of words per band (3 through 5), allows for a band weight and up to four cross sections: total, elastic, capture and fission. Total and elastic are always present (3); capture and fission may or may not be present (3 through 5).

1206
Start of data for the first evaluation.

The data for each evaluation includes a copy of the above five words from the evaluation map (for checking purposes), followed by the actual multiband parameters. The starting address specified in the evaluation map points to the beginning of the actual multiband parameters; the copy of the five words from the evaluation map PRECEDE this address.

For example, for the first evaluation the evaluation map specifies a starting address of 1211. This is preceded by the five words in addresses 1206 through 1210.

The order of evaluations is from lowest ZA to highest ZA, starting with the neutron, ZA = 1, up to ZA = 98252, the highest real ZA, and finally ending with the ENDL convention that Z = 99 means fission products.

The order of the data for each evaluation is from lowest energy group to highest (always 175 groups). For each group data is given for each cross section band (always 2 bands). For each band 3 through 5 parameters are given in the order: band weight, total, elastic, capture, fission. Weight, total and elastic are always given; capture and fission are option. Therefore the order of the data is: first group, first band, 3 through 5 parameters, first group, second band, 3 through 5 parameters, second group, first band, 3 through 5 parameters, etc. until parameters have been specified for the two bands of all 175 groups.

The data for each evaluation is immediately followed by data for the next evaluation. For example, the first evaluation has three parameters per band, for a total of 175 groups x 2 bands x 3 parameters = 1050 words. The actual data starts at address 1211 and extend through 2260. The next evaluation starts in address 2261: 2261 through 2265 are the copy of the five words from the evaluation map and the actual data starts of 2266 (this is the address in the evaluation map). This continues all the way to the end of the file.