A Compact ENDF (ACE) Format Specification

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1 Introduction

The ACE format consists of two *types* and many *classes* of data. The data are kept in an ACE Table. The term ACE Table and ACE file are often used interchangeably.

1.1 Types of ACE-Formatted Data

There are two types of ACE-formatted data; simply called Type 1 and Type 2.

Type 1 Standard formatted tables. These tables contain ASCII text and are machine independent; they are readable on every machine.

Type 2 Standard unformatted tables. These tables are binary and can be generated from the Type 1 files. They are more compact and faster to read than the Type 1 ACE Tables but are machine/platform dependent; they are not readable on every machine.

Traditionally Type 2 ACE files were more commonly used because they were smaller in size and faster to read. However due to the fact that they are not portable across machines and platforms they have fallen out of fashion.

1.2 Classes of ACE-Formatted Data

There are many classes of ACE-formatted data:

1. continuous-energy neutron (see Section 4),
2. discrete-reaction neutron,
3. neutron dosimetry (see Section 5),
4. $S(\alpha, \beta)$thermal (see Section 6),
5. continuous-energy photoatomic (see Section 7),
6. continuous-energy electron interaction,
7. continuous-energy photonuclear interaction,
8. multigroup-energy neutron, and
9. multigroup-energy photoatomic.

Each of these classes of data are described later in this document.

An ACE Table is an entity that contains evaluation-dependent data about one of the many classes of data for a specific material—an target isotope, isomer, or element. For a given ZAID, the data contained on a Type 1 and Type 2 tables are identical. Simulations run with one type of data should produce identical results as those run with the other type of data.

1.3 ACE Libraries

A collection of ACE data tables that derive from a single set of evaluation files are typically grouped together in a "library"—not to be confused from the evaluation library from which they derive. Multiple ACE data tables can concatenated into the same logical file on the computer, although this has fallen somewhat out of fashion due to the large amount of data on each ACE table derived from modern evaluation files. Applications that use ACE-formatted data should produce the same results regardless of whether the tables are contained in one logical file on the computer or spread across many.

2 ACE Tables

An ACE Table consists of a Header followed by an array (XSS) containing the actual data. The Header and XSS array are the same regardless of whether the ACE Table is Type 1 or Type 2. Each line in a Type 1 ACE Table is 80 characters or less.

2.1 ACE Header

The first section of an ACE Table is the Header. The ACE Header contains metadata[1] about the ACE Table. The Header consists of four parts:

1. Opening,
2. IZAW array,
3. NXS array, and
4. JXS array.

An example of an ACE Table Header (from ^{1}H in the ENDf71x library) is given in Figure 1 with each part highlighted a different color.

```
1  1001.80c    0.999167  2.5301E-08   12/17/12
2  H1 ENDF71x (jlconlin)  Ref. see jlconlin (ref 09/10/2012  10:00:53)      mat 125
3        0          0.         0          0.         0          0.         0          0.
4        0          0.         0          0.         0          0.         0          0.
5        0          0.         0          0.         0          0.         0          0.
6        0          0.         0          0.         0          0.         0          0.
7      17969       1001       590          3          0          1          1          0
8          0          1          1          0          0          0          0          0
9          1          0       2951       2954       2957       2960       2963       4352
10      4353       5644       5644       5644       6234       6235       6236       6244
11      6245       6245       6246      16721          0      16722          0          0
12         0          0          0          0          0      16723      16724      16725
```

Figure 1: Header example. The (Legacy) Opening (lines 1–2) is in red, the IZAW array (lines 3–6) is in blue, the NXS array (lines 7–8) is in teal, and the JXS array (lines 9–12) is in violet.

Legacy Header Opening There are two slightly different formats for the Header Opening. The most common one found is called here the Legacy Opening and is the one demonstrated in the Header example in Figure 1.

The Legacy Opening consists of several variables given over two 80-character lines. The variables and the Fortran format for reading the variable is given in Table 1

2.0.1 Header Opening

Don't forget the 2.0.1 Header Opening

[1] data about the data

Line	Variable	Format	Description
1	HZ	A10	ZAID (see Section 3.1)
1	AW	E12.0	atomic weight ratio
1	TZ	E12.0	temperature
1	—	1X	(blank space)
1	HD	A10	processing date
2	HK	A70	descriptive string
2	HM	A10	10-character material identifier

Table 1: Variables in the Legacy Opening part of the ACE Header.

Line	Variable	Format	Description
1	VERS	A10	version format string
1	HZ	A24	SZAID (see Section 3.2)
1	SRC	???	evaluation source
2	AW	E12.0	atomic weight ratio
2	TZ	E12.0	temperature
2	—	1X	(blank space)
2	HD	A10	processing date
2	N	I10	number of comment lines to follow
3–(N+2)	—	A70	comment lines

Table 2: Variables in the 2.0.1 Opening part of the ACE Header.

There is a limitation to the number of unique ZA IDs for a given ZA; 100 different IDs, in fact, for each class of ACE Table. To overcome this limitation, a new Header Opening was developed in 2013and updated a few years later to correct some errors. check this

```
2.0.0      1001.710nc              ENDFB-VII.1
0.999167 2.5301E-08 12/17/12     3
The next two lines are the first two lines of 'old-style' ACE.
  1001.80c    0.999167  2.5301E-08   12/17/12
H1 ENDF71x (jlconlin)  Ref. see jlconlin (ref 09/10/2012  10:00:53)      mat 125
```

Figure 2: Header Opening example. The Legacy Opening is shown in blue while the 2.0.1 Opening consists of the red and the blue portions.

Note that a Legacy Header Opening can be contained in the comment section of the 2.0.1 Header Opening. This was designed explicitly to allow backwards compatibility while application codes were modified to be able to handle. An example of this is shown in Figure 1. Codes that cannot read the 2.0.1 Header can be told (typically via an verify correctness xsdirentry) to start reading the ACE Table several lines after the beginning of the 2.0.1 Header.

provide reference

Following the Opening of the Header are three arrays, IZAW, NXS, and JXS respectively. They are each described below. Immediately following the JXS array is the XSSarray.

2.1.1 IZAW Array

The IZAW array follows on the lines immediately following the Header. It consists of 16 pairs of ZA's (`IZ`) and atomic weight ratios (`AW`). The `IZ` entries are still needed for $S(\alpha, \beta)$ Tables to indicate for which isotope(s) the scattering data are appropriate.

The 16 pairs of numbers are spread over 4 lines. The Fortran format for reading/writing the numbers on one line is: `4(I7,F11.0)`.

2.1.2 NXS Array

The NXS array comes on the 2 lines after the IZAW array. The NXS array has 16 integer elements; 8 on each line. The Fortran format for reading/writing the numbers on each line is: `8I9`. The first element of the NXS array indicates how many numbers are in the XSS array. The remainder of the NXS array elements (usually) indicate how many of different pieces of data there is.

2.1.3 JXS Array

The JXS array comes on the 4 lines after the NXS array. The JXS array has 32 integer elements; 8 on each line. The Fortran format for reading/writing the numbers on each line is: `8I9`. The JXS array contains indices to the XSS array where difference pieces of data begins.

The specific definition of the elements of the NXS and JXS arrays are dependent on the class of data in the Table and are defined in the section of this document that describes each class of data.[2] Note that not all elements of the arrays are (currently) being used, allowing for future expansion.

2.2 The XSS Array

After the ACE Header comes the XSS array. It is typically *very* large with hundreds of thousands of elements. It is broken up into blocks with the blocks being dependent on the class of data that is contained in the table. The description and definition of each of these blocks can be found in the descriptions later in this document.

The data is written with 4 floating-point numbers on each 80-character line. All data in the XSS array can be read using the Fortran format: `4E20.0` for each line.

[2]See, for example, Table 3 and Table 4.

```
2.0.0      1001.710nc              ENDFB-VII.1
0.999167 2.5301E-08 12/17/12     3
The next two lines are the first two lines of 'old-style' ACE.
  1001.80c    0.999167  2.5301E-08   12/17/12
H1 ENDF71x (jlconlin)  Ref. see jlconlin (ref 09/10/2012  10:00:53)      mat 125
1.00000000000E-11   1.03125000000E-11   1.06250000000E-11   1.09375000000E-11
1.12500000000E-11   1.15625000000E-11   1.18750000000E-11   1.21875000000E-11
1.25000000000E-11   1.28125000000E-11   1.31250000000E-11   1.34375000000E-11
1.37500000000E-11   1.43750000000E-11   1.50000000000E-11   1.56250000000E-11
1.62500000000E-11   1.68750000000E-11   1.75000000000E-11   1.81250000000E-11
1.87500000000E-11   1.93750000000E-11   2.00000000000E-11   2.09375000000E-11
2.18750000000E-11   2.28125000000E-11   2.37500000000E-11   2.46875000000E-11
2.56250000000E-11   2.65625000000E-11   2.75000000000E-11   2.84375000000E-11
2.93750000000E-11   3.03125000000E-11   3.12500000000E-11   3.21875000000E-11
3.31250000000E-11   3.40625000000E-11   3.50000000000E-11   3.59375000000E-11
```

Figure 3: ACE Header with beginning of XSS array for ^{1}H from the ENDF71x library. Note this uses the 2.0.1 Header with backwards compatibility with the Legacy Header.

3 Unique ACE Table Identifier

This needs to be done.

Each ACE Table needs to have an identifier to uniquely distinguish the data that is contained in the Table.

3.1 ZAID

3.2 SZAID

With the introduction of the 2.0.1 ACE Header, the identifier was modified to better specify the metastable state of the material as well as expand the available space for identifiers.

The new identifier is referred to as a SZAID[3].

[3] pronounced "ess-ZAID"

4 Continuous-Energy and Discrete Neutron Transport Tables

The format of individual blocks found on neutron transport tables is identical for continuous-energy and discrete-reaction ACE Tables; the format for both are described in this section. The blocks of data are:

1. **ESZ Block**—contains the main energy gid for the Table and the total, absorption, and elastic cross sections as wella s the average heating numbers. The ESZ Block block always exists. See Table 5.
2. **NU Block**—contains prompt, delayed and/or total $\overline{\nu}$ as a function of incident neutron energy. The NU Block exists only for fissionable isotopes; that is, if `JXS(2)`$\neq 0$. See Table 6.
3. **MTR Block**—contains a list of ENDF MT numbers for all neutron reactions other than elastic scattering. The MTR Block exists for all isotopes that have reactions other than elastic scattering; that is, all isotopes with `NXS(4)`$\neq 0$. See Table 7.
4. **LQR Block**—contains a list of kinematic Q-values for all neutron reactions other than elastic scattering. The LTR Block exists if `NXS(4)`$\neq 0$. See Table 8.
5. **TYR Block**—contains information about the type of reaction for all neutron reactions other than elastic scattering. Information for each reaction includes the number of secondary neutrons and whether secondary neutron angular distributions are in the laboratory or center-of-mass system. The TYR Block exists if `NXS(4)`$\neq 0$. See Table 9.
6. **LSIG Block**—contains a list of cross section locators for all neutron reacitons other than elastic scattering. The LSIG Block exists if `NXS(4)`$\neq 0$. See Table 10
7. **SIG Block**—contains cross sections for all reactions other than elastic scattering. The SIG Block exists if `NXS(4)`$\neq 0$. See Table 11.
8. **LAND Block**—contains a list of angular-distribution locators for all reactions producing secondary neutrons. The LAND Block always exists. See Table 12.
9. **AND Block**—contains list angular distributions for all reactions producing secondary neutrons. The AND Block always exists. See Table 13.
10. **LDLW Block**—contains a list of energy distributions for all reactions producing secondary neutrons except for elastic scattering. The LDLW Block exists if `NXS(5)`$\neq 0$. See Table 14.
11. **DLW Block**—contains energy distributions for all reactions producing secondary neutrons except for elastic scattering. The DLW Block exists if `NXS(5)`$\neq 0$. See Table 15.
12. **GPD Block**—contains the total photon production cross section tabulated on the ESZ energy grid and a 30$\times$ matrix of secondary photon energies. The GPD Block exists only for those older evaluations that provide coupled neutron/photon information; that is, if `JXS(12)`$\neq 0$. See Table 16.
13. **MTRP Block**—contains a list of MT numbers for all photon production reactions. The term "photon production reaction" is used for any information describing a specific neutron-in, photon-out reaction. The MTRP Block exists if `NXS(6)`$\neq 6$.

See Table 17.

14. **LSIGP Block**—contains a list of cross section locators for all photon production reactions. The LSIGP Block exists if `NXS(6)`$\neq 0$. See Table 18.
15. **SIGP Block**—contains cross sections for all photon production reactions. The SIGP Block exists if `NXS(6)`$\neq 0$. See Table 19.
16. **LANDP Block**—contains a list of angular-distribution locators for all photon production reactions. The LANDP Block exist if `NXS(6)`$\neq 0$. See Table 20
17. **ANDP Block**—contains photon angular distributions for all photon production reactions. The ANDP Block exists if `NXS(6)`$\neq 0$. See Table 21.
18. **LDLWP Block**—contains a list of energy-distribution locators for all photon production reactions. The LDLWP Block exists if `NXS(6)`$\neq 0$. See Table 22.
19. **DLWP Block**—contains photon energy distributions for all photon production reactions. The DLWP Block exists if `NXS(6)`$\neq 0$. See Table 23.
20. **YP Block**—contains a list of MT identifiers of neutron reaction cross sections required as photon production yield multipliers. The YP Block exists if `NXS(6)`$\neq 0$. See Table 24.
21. **FIS Block**—contains the total fission cross section tabulated on the ESZ energy grid. The FIS Block exists if `JXS(21)`$\neq 0$. See Table 25.
22. **UNR Block**—contains the unresolved resonance range probability tables. The UNR Block exists if `JXS(23)`$\neq 0$. See Table 26.

4.1 NXS Array

Table 3: NXS array element definitions for NXS ACE Table.

Element	Name	Description
1	—	Length of second block of data (XSS array)
2	ZA	$1000 * Z + A$
3	NES	Number of energies
4	NTR	Number of reactions excluding elastic scattering
5	NR	Number of reactions having secondary neutrons excluding elastic scattering
6	NTRP	Number of photon production reactions
	...	
8	NPCR	Number of delayed neutron precurser families
	...	
15	NT	Number of PIKMT reaction
16	—	0=normal photon production -1=do not produce photons

Does NXS[15] apply to every type of data, or just fast tables?

4.2 JXS Array

Table 4: JXS array element definitions for JXS ACE Table.

Element	Name	Location Description
1	ESZ	Energy table
2	NU	Fission ν data
3	MTR	`MT` array
4	LQR	Q-value array
5	TYR	Reaction type array
6	LSIG	Table of cross section locators
7	SIG	Cross sections
8	LAND	Table of angular distribution locators
9	AND	Angular distributions
10	LDLW	Table of energy distribution locators
11	DLW	Energy distributions
12	GPD	Photon production data
13	MTRP	Photon production `MT` array
14	LSIGP	Table of photon production cross section locators
15	SIGP	Photon production cross sections
16	LANDP	Table of photon production angular distribution locators
17	ANDP	Photon production angular distributions
18	LDLWP	Table of photon production energy distribution locators
19	DLWP	Photon production energy distributions
20	YP	Table of yield multipliers
21	FIS	Total fission cross section
22	END	Last word of this table
23	LUNR	Probability tables
24	DNU	Delayed $\overline{\nu}$ data
25	BDD	Basic delayed data (λ's, probabilities)
26	DNEDL	Table of energy distribution locators
27	DNED	Energy distributions
	...	
32	—	

4.3 Format of Individual Data Blocks

Table 5: ESZ Block.

Location in XSS	Parameter	Description
S_{ESZ}	$E(l), l = 1, \ldots N_E$	Energies
JXS(1) + N_E	$\sigma_t(l), l = 1, \ldots N_E$	Total cross section

Note: S_{ESZ} is index of the XSS array where the ESZ Block starts; JXS(1). where N_E is the number of energy energy points NXS(3).

Table 6: NU Block.

Location in XSS	Parameter	Description

Table 7: MTR Block.

Location in XSS	Parameter	Description

Table 8: LQR Block.

Location in XSS	Parameter	Description

Table 9: TYR Block.

Location in XSS	Parameter	Description

Table 10: LSIG Block.

Location in XSS	Parameter	Description

Table 11: SIG Block.

Location in XSS	Parameter	Description

Table 12: LAND Block.

Location in XSS	Parameter	Description

Table 13: AND Block.

Location in XSS	Parameter	Description

Table 14: LDLW Block.

Location in XSS	Parameter	Description

Table 15: DLW Block.

Location in XSS	Parameter	Description

Table 16: GPD Block.

Location in XSS	Parameter	Description

Table 17: MTRP Block.

Location in XSS	Parameter	Description

Table 18: LSIG Block.

Location in XSS	Parameter	Description

Table 19: SIG Block.

Location in XSS	Parameter	Description

Table 20: LANDP Block.

Location in XSS	Parameter	Description

Table 21: ANDP Block.

Location in XSS	Parameter	Description

Table 22: LDLWP Block.

Location in XSS	Parameter	Description

Table 23: DLWP Block.

Location in XSS	Parameter	Description

Table 24: YP Block.

Location in XSS	Parameter	Description

Table 25: FIS Block.

Location in XSS	Parameter	Description

Table 26: UNR Block.

Location in XSS	Parameter	Description

Element	Name	Description
1	—	Length of second block of data (XSS array)
2	ZA	$1000 * Z + A$
3	—	
4	NTR	Number of reactions
	...	
16	—	

Table 27: NXS array element definitions for neutron dosimetry ACE Table.

Element	Name	Location Description
1	LONE	First word of table
2	—	
3	MTR	`MT` array
	...	
6	LSIG	Table of cross section locators
7	SIGD	Cross sections
	...	
22	END	Last word of this table
	...	
32	—	

Table 28: JXS array element definitions for neutron dosimtry ACE Table.

5 Neutron Dosimetry

5.1 NXS Array

5.2 JXS Array

Element	Name	Description
1	—	Length of second block of data (XSS array)
2	IDPNI	Inelastic scattering mode
3	NIL	Inelastic dimensioning parameter
4	NIEB	Number of inelastic exiting energies
5	IDPNC	Elastic scattering mode
6	NCL	Elastic dimensioning parameter
7	IFENG	Secondary energy mode
	...	
16	—	

Table 29: NXS array element definitions for thermal scattering ACE Table.

Element	Name	Location Description
1	ITIE	Inelastic energy table
2	ITIX	Inelastic cross sections
3	ITXE	Inelastic energy/angle distributions
4	ITCX	Elastic cross sections
5	ITCA	Elastic angular distributions
	...	
32	—	

Table 30: JXS array element definitions for thermal scattering ACE Table.

6 Thermal Scattering $S(\alpha, \beta)$

6.1 NXS Array

6.2 JXS Array

7 Continuous-Energy Photon

7.1 NXS Array

Table 31: NXS array element definitions for NXS ACE Table.

Element	Name	Description
1	—	Length of second block of data (XSS array)
2	Z	Atomic number
3	NES	Number of energies
4	NFLC	Length of the flourescence data divided by 4
5	NSH	Number of electron shells[a]
	...	
16	—	

[a] mcplib03 and later, older libraries don't use this option.

7.2 JXS Array

Table 32: JXS array element definitions for JXS ACE Table.

Element	Name	Location Description
1	ESZG	Energy table
2	JINC	Incoherent form factors
3	JCOH	Coherent form factors
4	JFLO	Fluorescence data
5	LHNM	Heating numbers
6	LNEPS	Number of electrons per shell[a]
7	LBEPS	Binding energy per shell[a]
8	LPIPS	Probability of interaction per shell[a]
9	LSWD	Array of offsets to the shell-wise data [a]
10	SWD	Shell-wise data in PDF and CDF form[a]
	...	
32	—	

[a] mcplib03 and later, older libraries don't use this option.