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An Electron/Photon/Relaxation Data Library for MCNP6

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ABSTRACT

The capabilities of the MCNP6 Monte Carlo code in simulation of electron transport, photon transport, and atomic relaxation have recently been significantly expanded. The enhancements include not only the extension of existing data and methods to lower energies, but also the introduction of new categories of data and methods. Support of these new capabilities has required major additions to and redesign of the associated data tables. In this paper we present the first complete documentation of the contents and format of the new electron-photon-relaxation data library now available with the initial production release of MCNP6.

I. INTRODUCTION

The recent release of the Los Alamos Monte Carlo transport code MCNP6[(1)] marks the culmination of several years of work to combine all of the capabilities of the earlier MCNP5[(2)] and MCNPX[(3)] codes, to improve the resulting code system, and to include a number of new features as well. One of these new features is a major expansion of the coupled electron/photon transport capability.[(4)] This work relies on the availability of a set of libraries of photon, electron, and atomic structure data developed over many years by D. E. Cullen and collaborators.[(5–7)] The then-latest versions of those libraries were officially adopted in the ENDF/B VI.8 release of the Evaluated Nuclear Data File[(8)] and are now in use in MCNP6. (The latest version of the libraries, EPICS2014,[(9)] has not yet been incorporated into the MCNP6 system, but will be the basis for the eventual next release of **eprdata**.) To make the new data available to the code using standard MCNP6 data-handling methods, a new library in ACE (A Compact ENDF) format has been designed. This library, called **eprdata12**, is available with the first production release of MCNP6. In this paper we present a description of the extended data and a full specification of the format of this newly created ACE library.

The categories of data in the new library constitute a significant superset of those in earlier photoatomic libraries, such as **mcplib04**.[(10)] Some of the data merely extend familiar information to a wider energy range using the existing format, but with more data points. A few sets of data are actually identical to those in the existing library. However, by far the largest part of the new library consists of types of data that are entirely new to MCNP. Therefore a new, extended format for the library was required, and for certain technical reasons of implementation, discussed below, the resulting new library is usable only by the current version of MCNP6 (the first production release of that code), and not by the earlier codes, MCNP5 and MCNPX.

At the highest level of view, a data table from **eprdata12** will be quite recognizable to the data user, as it follows the standard (traditional) overall form of ACE-format tables. Such a table consists of two consecutive blocks of data. The first, containing various identifiers, counters, and locators for data, consists of twelve lines of text, as follows.

Line 1:	ZAID	AW(0)	TZ	DATE		(A10,2E12.0,1X,A10)
Line 2:	HK	HM				(A70,A10)
Lines 3–6:	IZ(1)	AW(1)	…	IZ(4)	AW(4)	(4(I7,F11.0))
	IZ(5)	AW(5)	…	IZ(8)	AW(8)	(4(I7,F11.0))
	IZ(9)	AW(9)	…	IZ(12)	AW(12)	(4(I7,F11.0))
	IZ(13)	AW(13)	…	IZ(16)	AW(16)	(4(I7,F11.0))
Lines 7–8:	NXS(1)		…		NXS(8)	(8I9)
	NXS(9)		…		NXS(16)	(8I9)
Lines 9–12:	JXS(1)		…		JXS(8)	(8I9)
	JXS(9)		…		JXS(16)	(8I9)
	JXS(17)		…		JXS(24)	(8I9)
	JXS(25)		…		JXS(32)	(8I9)

Here ZAID is the element identifier in the customary 10-character form (e.g. 26000.12p). AW(0) is an average atomic weight for the element, TZ is a temperature (always zero for photon and electron tables), and the strings DATE, HK, and HM are used to identify the specific table. The arrays IZ(1:16) and AW(1:16) can be used to provide isotope-specific atomic weights, but are always zero for photon and electron tables. The NXS(1:16) array contains two pieces of identifying information and various counters applying to the data of the table. The JXS(1:32) array contains locators that are used to find particular sub-blocks within the second block of data. The parenthesized expressions at the end of each line are the FORTRAN-readable formats for the items in the first block.

The second block of data, immediately following the information above, consists of a simple list of floating-point numbers, four to a line in FORTRAN-readable format (4E20.0). The number of items in this list is given in the first block as NXS(1). The data table ends after the last line needed to provide this list of data items. As is familiar from other ENDF-based libraries, any number of tables may be concatenated to form an ACE-format library. In particular, **eprdata12** contains the new ENDF/B-VI.8-based tables for the elements from $Z = 1 \ldots 100$.

II. CONTENTS OF AN ELECTRON-PHOTON-RELAXATION DATA TABLE

In this section we provide a complete description of the structure and contents of the new data tables. We present this information in four parts, in Tables 1–4 below. The first of these, Table 1, defines each element of the NXS(1:16) array and identifies the special counters N_γ, N_F, N_D, N_S, N_e, N_{XL}, N_A, N_B, and N_{BL} that will be used to clarify the locations of various data blocks, especially in Table 4.

TABLE 1. Definition of Elements in the NXS array.

NXS(1)	Length of second block of data.
NXS(2)	Z (the atomic number).
NXS(3) = N_γ	Number of photon energies (common grid) for all cross sections and heating.
NXS(4) = N_F	Length of (old method) fluorescence data divided by 4.
NXS(5) = N_D	Number of shells (for Compton Doppler broadening).
NXS(6) = 1	New format flag.
NXS(7) = N_S	Number of subshells for photoelectric and electron impact ionization.
NXS(8) = N_e	Number of electron energies (separate common grid) for all cross sections.
NXS(9)= N_{XL}	Length of {energy, energy-loss} table for electron excitation.
NXS(10)= N_A	Number of energies for which there are electron elastic angular tables.
NXS(11)= N_B	Number of energies for which there are bremsstrahlung photon energy tables.
NXS(12)= N_{BL}	Length of {energy, energy-loss} table for electron bremsstrahlung.
NXS(13…16)	Not used.

Table 2 provides the definitions of the JXS(1:32) array of locators for the various sub-blocks in the second block of data. Two additional special counters, N_{inc} and N_{coh}, are also defined here, and are used to help locate form factor data as indicated in Table 4.

TABLE 2. Definition of Elements in the JXS array.

JXS(1)	Relative start of data block (location of photon energies).
JXS(2)	Location of photon incoherent form factors. $N_{inc} = \big(JXS(3) - JXS(2)\big)/2$

JXS(3)	Location of photon coherent form factor. $N_{coh} = \big(JXS(4) - JXS(3)\big)/3$
JXS(4)	Location of (old method) fluorescence data.
JXS(5)	Location of heating numbers.
JXS(6)	Location of number of electrons in each shell (for Compton Doppler broadening).
JXS(7)	Location of shell binding energies (for Compton Doppler broadening).
JXS(8)	Location of shell probabilities (for Compton Doppler broadening).
JXS(9)	Location of relative locations of shell data (for Compton Doppler broadening).
JXS(10)	Location of shell data (for Compton Doppler broadening).
JXS(11)	Location of subshell designators (ENDF representation).
JXS(12)	Location of number of electrons in each subshell.
JXS(13)	Location of binding energies for each subshell.
JXS(14)	Location of probabilities for Compton-induced vacancies.
JXS(15)	Location of number of transitions (to fill a vacancy) for each subshell.
JXS(16)	Location of subshell photoelectric cross sections.
JXS(17)	Location of offsets to atomic relaxation transition data.
JXS(18)	Location of atomic relaxation transition data.
JXS(19)	Location of electron energies (separate common grid for electron cross sections).
JXS(20)	Location of average energy-loss table for electron excitation.
JXS(21)	Location of electron elastic angular distribution information.
JXS(22)	Location of electron elastic angular distribution tables.
JXS(23)	Location of electroionization table information.
JXS(24)	Location of bremsstrahlung table information.
JXS(25)	Location of bremsstrahlung photon energy spectrum tables.
JXS(26)	Location of bremsstrahlung electron average energy-loss table.
JXS(27…32)	Not used.

It is convenient (and conventional) to subdivide the second block of data into a consecutive set of sub-blocks in order to clarify the purpose and contents of the various parts of the block. Table 3 provides this subdivision and also indicates the starting point of each sub-block in terms of the JXS(1:32) array. At the end of Table 3 there are notes covering a variety of technical points of which users and developers may need to be aware.

TABLE 3. (Sub)Blocks within the Second Block of Data.

Block	Start	Contents
ESZG	JXS(1)	Natural logarithms of the energies in the common photon energy grid and of the incoherent, coherent, total photoelectric, and pair-production cross sections. As in previous libraries, the cross section for triplet production (photon creating one positron and two electrons) is included in the cross section for pair production, and no distinction is made between the two processes. See Note 1 below for some implications of the logarithmic storage.
JINCE	JXS(2)	Incoherent scattering form factors: element-specific modifiers of the Klein-Nishina cross section. See Note 2 below.
JCOHE	JXS(3)	Coherent scattering form factors: element-specific modifier of the Thomson cross section. See Note 2 below.
JFLO	JXS(4)	Fluorescence data. This block exists if NXS(4) > 0. These data have exactly the same values in the same format as the JFLO blocks in previous libraries, so that backwardly-compatible investigations can reproduce earlier results.
LHNM	JXS(5)	Average heating numbers, tabulated on the same energy grid that is given in the ESZG block.
LNEPS	JXS(6)	This block and the four following blocks are duplicates of the corresponding blocks in earlier libraries. They contain data necessary for the Compton Doppler broadening model that affects the energy distribution from incoherent scattering. The LNEPS block contains the number of electrons per shell for the Doppler broadening model.
LBEPS	JXS(7)	Shell binding energies for the Doppler broadening model.
LPIPS	JXS(8)	Probabilities of interaction for shells for the Doppler broadening model. See Note 3 below.

LSWD	JXS(9)	Relative locations of the data for each shell for the Doppler broadening model.
SWD	JXS(10)	Doppler broadening data. The detailed format is shown in Table 3 below.
SUBSH	JXS(11)	Information about the atomic electron subshells of the element as given in the ENDF/B VI.8 release. There are five sets of data in this block: the ENDF designators for the subshells, the electron populations by subshell, the subshell binding energies, the subshell vacancy cumulative probabilities for incoherent (Compton) scattering, and the number of possible transitions to fill a vacancy in each subshell. With the new extended data, at least the K shell always exists for every element.
SPHEL	JXS(16)	Natural logarithms of the photoelectric cross sections for each subshell, tabulated on the same common energy grid given at the beginning of the ESZG block. See Note 1 below.
RELO	JXS(17)	Offsets to relaxation data for each subshell.
XPROB	JXS(18)	Identities, line energies, and cumulative probabilities of atomic transitions, listed for each possible transition to fill a subshell vacancy, for each existing subshell. As previously mentioned, at least one subshell (the K shell) always exists, but it is not necessarily the case that allowed and tabulated transitions exist to fill a vacancy in a given subshell. The XPROB block exists only when there is at least one tabulated transition for at least one subshell (in practice for elements with $Z \geq 6$). See Note 4 and Table 4 for the specific format.
ESZE	JXS(19)	Electron energies (in a separate common grid different from the one in the ESZG block) and corresponding tabulations of the electron total, elastic, bremsstrahlung, excitation, and total electroionization cross sections, and subshell-specific electroionization cross sections for each provided subshell for the element. In contrast to photon data, these energies and cross sections are saved as actual values, not as logarithms.
EXCIT	JXS(20)	Energies for tabulating electron excitation, and the corresponding average excitation energy loss.
ELASI	JXS(21)	Information for elastic scattering: energies for which there are elastic angular tables, the lengths of, and offsets to those tables.

ELAS	JXS(22)	Data for elastic scattering angular distributions, given as tabulations of cosines of scattering angles and corresponding tabulations of cumulative probabilities for the associated angular bins, with one such pair of tabulations for each angular table. See Note 5 below.
EION	JXS(23)	This is the most complex of the new data blocks. It begins with lists by subshell of the number of electroionization (knock-on electron) tables, the locations of information about these tables, and the locations of the tables themselves. Then for each subshell in turn, these is a list of energies at which each table is to be applied, a list of lengths of the tables, and a list of offsets to the tables, followed a repeated sub-block for each table of the subshell containing a tabulation of the possible knock-on electron energies and a tabulation of the cumulative probabilities of those energies. Table 4, below, shows the exact format of the EION block.
BREMI	JXS(24)	Information for bremsstrahlung photon energy sampling data: a list of electron energies for which there are bremsstrahlung energy tables, a list of lengths of those tables, and a list of offsets to the tables.
BREME	JXS(25)	For each bremsstrahlung energy table in turn, this block contains a tabulation of possible bremsstrahlung photon energies and the corresponding cumulative probabilities for those energies.
BREML	JXS(26)	Energies for tabulating bremsstrahlung energy loss, and the corresponding average energy remaining with the electron following the interaction. See Note 6 below.

Note 1. The photon energies and cross sections contained in the ESZG and SPHEL blocks are stored as the natural logarithms of their actual values for more efficient access in the transport code, which uses logarithmic interpolation among these quantities. This creates a specific problem in data handling, since some of the cross sections can have the value zero in certain energy ranges. Rather than choosing a flag to represent $-\infty = \ln(0)$, the traditional convention is that a zero value for any entry in the ESZG and SPHEL blocks is interpreted as an actual zero for the value, and not as $0 = \ln(1)$. This requires an extra test in the code to detect this special case, but it is still considered to be more efficient than converting all values to logarithms before each interpolation. (There are also implications for the developer of data libraries, regarding energies or cross sections that could have the value unity.)

Note 2. The form-factor data in the JINCE and JCOHE blocks are analogous to the information contained in the JINC and JCOH blocks found in earlier photoatomic libraries (the **mcplib** series). Those earlier libraries took advantage of certain simplifications that resulted from the limitations of the existing data. However, the extended and generalized data available[(11)] with ENDF/B VI.8 require a change in format. The new format is not correctly readable by earlier versions of the code. MCNP6, of course, has been designed to read either the old format or the new one, but this format difference constitutes the first of two issues that prevent earlier codes (MCNP5 and MCNPX) from successfully using the new **eprdata12** library.

Note 3. The LPIPS block has been the source of some confusion in the past. It actually contains differential data: probabilities of interaction for each shell, normalized so that the sum of the probabilities should be unity. Unfortunately earlier versions of the code treated these probabilities as cumulative,[(12)] leading to at least slightly wrong results for Doppler broadening for any element with more than one shell, namely every element beyond Helium. This problem has recently been addressed in two ways. (1) First, two new photoatomic libraries, **mcplib63** and **mcplib84**, have been generated to replace **mcplib03** and **mcplib04**, respectively. These differ from their predecessors only in that the probabilities in the LPIPS block have been converted to cumulative form. Therefore users of earlier codes (MCNP5 and MCNPX) can switch to these new libraries and obtain more theoretically correct results from Compton Doppler broadening. (2) Second, the current version of the code, MCNP6, has been given the ability to distinguish between differential and cumulative probabilities in the LPIPS block and to convert automatically to the cumulative form. Therefore users of MCNP6 will obtain the improved results regardless of the form of the LPIPS block in the library. The new electron-photon-relaxation library **eprdata12** was finalized before the discovery of this issue, and so still contains differential data in the LPIPS block. This is the second of two issues that prevent the new data library from being safely used with the earlier codes, since only MCNP6 has the ability to convert the differential data to the desired cumulative form.

Note 4. The XPROB block consists of sets of four numbers, one set for each transition capable of filling an electron vacancy in a subshell, for each subshell of the element. Each such set contains the numbers **{** *designator 1*, *designator 2*, *energy*, *probability* **}**. This description makes use of ENDF definitions to specify the transition. *Designator 1* is the standard ENDF designator for the subshell from which an electron will "move" to fill the current vacancy. If that transition is radiative (emitting only a photon) then *designator 2* is zero. If instead the transition is non-radiative (emitting an Auger or Coster-Kronig electron) then *designator 2* is the ENDF designator of the subshell from which the emitted electron will be ejected, leaving two vacancies in the atom. Of course *energy* is the energy of the emitted photon or electron, and *probability* is

the cumulative probability that this particular transition occurs.

Note 5. The representation of electron elastic angular distributions suffers from a limitation of the ENDF format, which is insufficiently precise to resolve satisfactorily the strong forward peak of the scattering distribution. This results in some uncertainty and unsolved problems in the current model for the electron elastic scattering. This issue is under active investigation.

Note 6. The intention of the evaluators[13] was that the average energy loss to bremsstrahlung should be tabulated as a function of the electron energy at the bremsstrahlung event. This was inadvertently reversed to the form described in the BREML block (average energy remaining with the electron after the bremsstrahlung event at the tabulated electron energy), and appears in that form in the ENDF/B VI.8 evaluation. For consistency with the ENDF release, this definition is retained in **eprdata12**, although the question may be revisited if further development of the data library should be required in the future. (At the time of writing, MCNP6 does not make any use of the data in the BREML block.)

Finally, in Table 4 we conclude by providing an explicit representation of the information in the second data block, including notation, definitions, starting locations, and ending locations for each group of data as they occur in the data block.

TABLE 4. Map of the Contents of the Second Block of Data.

$\ln E_\gamma\,(1)$ $JXS(1)$	Logarithms of photon energies (common grid).	... $\ln E_\gamma\,(N_\gamma)$ $JXS(1)+N_\gamma-1$
$\ln \sigma_{inc}\,(1)$ $JXS(1)+N_\gamma$	Logarithms of incoherent scattering cross sections.	... $\ln \sigma_{inc}\,(N_\gamma)$ $JXS(1)+2\cdot N_\gamma-1$
$\ln \sigma_{coh}\,(1)$ $JXS(1)+2\cdot N_\gamma$	Logarithms of coherent scattering cross sections.	... $\ln \sigma_{coh}\,(N_\gamma)$ $JXS(1)+3\cdot N_\gamma-1$
$\ln \sigma_{phel}\,(1)$ $JXS(1)+3\cdot N_\gamma$	Logarithms of total photoelectric cross sections.	... $\ln \sigma_{phel}\,(N_\gamma)$ $JXS(1)+4\cdot N_\gamma-1$
$\ln \sigma_{pair}\,(1)$ $JXS(1)+4\cdot N_\gamma$	Logarithms of pair-production cross sections (pair and triplet combined).	... $\ln \sigma_{pair}\,(N_\gamma)$ $JXS(1)+5\cdot N_\gamma-1$
$X_{inc}(1)$ $JXS(2)$	Independent variable for photon incoherent form factors.	... $X_{inc}(N_{inc})$ $JXS(2)+N_{inc}-1$

$FF_{inc}(1)$ $JXS(2) + N_{inc}$	Incoherent form factors.	... $FF_{inc}(N_{inc})$ $JXS(2) + 2 \cdot N_{inc} - 1$
$X_{coh}(1)$ $JXS(3)$	Independent variable for photon coherent form factors.	... $X_{coh}(N_{coh})$ $JXS(3) + N_{coh} - 1$
$FFC_{coh}(1)$ $JXS(3) + N_{coh}$	Coherent form factors (cumulative).	... $FFC_{coh}(N_{coh})$ $JXS(3) + 2 \cdot N_{coh} - 1$
$FFD_{coh}(1)$ $JXS(3) + 2 \cdot N_{coh}$	Coherent form factors (differential).	... $FFD_{coh}(N_{coh})$ $JXS(3) + 3 \cdot N_{coh} - 1$
$BE_{old}(1)$ $JXS(4)$	Shell binding energies (old fluorescent method).	... $BE_{old}(N_F)$ $JXS(4) + N_F - 1$
$EJ_{old}(1)$ $JXS(4) + N_F$	Shell ejection probabilities (old fluorescent method).	... $EJ_{old}(N_F)$ $JXS(4) + 2 \cdot N_F - 1$
$Y_{old}(1)$ $JXS(4) + 2 \cdot N_F$	Yields (old fluorescent method).	... $Y_{old}(N_F)$ $JXS(4) + 3 \cdot N_F - 1$
$E_{old}(1)$ $JXS(4) + 3 \cdot N_F$	Line energies (old fluorescent method).	... $E_{old}(N_F)$ $JXS(4) + 4 \cdot N_F - 1$
$H(1)$ $JXS(5)$	Average heating numbers.	... $H(N_\gamma)$ $JXS(5) + N_\gamma - 1$
$EP_{Dopp}(1)$ $JXS(6)$	Shell electron populations (for Compton Doppler broadening).	... $EP_{Dopp}(N_D)$ $JXS(6) + N_D - 1$
$BE_{Dopp}(1)$ $JXS(7) = JXS(6) + N_D$	Shell binding energies (for Compton Doppler broadening).	... $BE_{Dopp}(N_D)$ $JXS(7) + N_D - 1$
$PR_{Dopp}(1)$ $JXS(8) = JXS(6) + 2 \cdot N_D$	Shell probabilities (for Compton Doppler broadening).	... $PR_{Dopp}(N_D)$ $JXS(8) + N_D - 1$
$LOC_{Dopp}(1) = 1$ $JXS(9) = JXS(6) + 3 \cdot N_D$	Relative locations of shell data. $LOC_{Dopp}(i+1) = LOC_{Dopp}(i) + 95$.	... $LOC_{Dopp}(N_D)$ $JXS(9) + N_D - 1$

$DATA_{Dopp}(1,1)$ $JXS(10)$	Doppler data for shell 1 (always exists).	... $DATA_{Dopp}(95,1)$ $JXS(10)+94$
$DATA_{Dopp}(1,2)$ $JXS(10)+LOC_{Dopp}(2)-1$	Doppler data for shell 2 (if present).	... $DATA_{Dopp}(95,2)$ $JXS(10)+LOC_{Dopp}(2)+93$
⋮		
$DATA_{Dopp}(1,N_D)$ $JXS(10)+LOC_{Dopp}(N_D)-1$	Doppler data for shell N_D (if present).	... $DATA_{Dopp}(95,N_D)$ $JXS(10)+LOC_{Dopp}(N_D)+93$
$ENDF(1)$ $JXS(11)$	ENDF designators for the subshells.	... $ENDF(N_S)$ $JXS(11)+N_S-1$
$EP(1)$ $JXS(12)=JXS(11)+N_S$	Subshell electron populations.	... $EP(N_S)$ $JXS(12)+N_S-1$
$BE(1)$ $JXS(13)=JXS(11)+2\cdot N_S$	Subshell binding energies.	... $BE(N_S)$ $JXS(13)+N_S-1$
$CV(1)$ $JXS(14)=JXS(11)+3\cdot N_S$	Subshell vacancy probabilities (from Compton scattering).	... $CV(N_S)$ $JXS(14)+N_S-1$
$NT(1)$ $JXS(15)=JXS(11)+4\cdot N_S$	Number of transitions to fill a vacancy in each subshell.	... $NT(N_S)$ $JXS(15)+N_S-1$
$\ln\sigma_{phel}^{1}(1)$ $JXS(16)$	Logarithms of photoelectric XS for subshell 1 (K always exists).	... $\ln\sigma_{phel}^{1}(N_\gamma)$ $JXS(16)+N_\gamma-1$
$\ln\sigma_{phel}^{2}(1)$ $JXS(16)+N_\gamma$	Logarithms of photoelectric cross sections for subshell 2 (if present).	... $\ln\sigma_{phel}^{2}(N_\gamma)$ $JXS(16)+2\cdot N_\gamma-1$
⋮		
$\ln\sigma_{phel}^{N_S}(1)$ $JXS(16)+(N_S-1)\cdot N_\gamma$	Logarithms of photoelectric cross sections for subshell N_S (if present).	... $\ln\sigma_{phel}^{N_S}(N_\gamma)$ $JXS(16)+N_S\cdot N_\gamma-1$
$OFF_{rel}(1)$ $JXS(17)$	Offsets to subshell relaxation data. $OFF_{rel}(1)=0$	... $OFF_{rel}(N_S)$ $JXS(17)+N_S-1$

Relaxation data for subshell 1, transition 1 (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)$	$JXS(18)+1$	$JXS(18)+2$	$JXS(18)+3$

Relaxation data for subshell 1, transition $t = 2$ (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)+4\cdot(t-1)$	… $+1$	… $+2$	… $+3$

⋮

Relaxation data for subshell 1, transition $NT(1)$ (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)+4\cdot(NT(1)-1)$	… $+1$	… $+2$	… $+3$

Relaxation data for subshell 2, transition 1 (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)+OFF_{rel}(2)$	… $+1$	… $+2$	… $+3$

Relaxation data for subshell 2, transition $t = 2$ (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)+OFF_{rel}(2)+4\cdot(t-1)$	… $+1$	… $+2$	… $+3$

⋮

Relaxation data for subshell 2, transition $NT(2)$ (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)+OFF_{rel}(2)+4\cdot(NT(2)-1)$	… $+1$	… $+2$	… $+3$

⋮

Relaxation data for subshell N_S, transition 1 (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18)+OFF_{rel}(N_S)$	… $+1$	… $+2$	… $+3$

Relaxation data for subshell N_S, transition $t = 2$ (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18) + OFF_{rel}(N_S) + 4 \cdot (t-1)$	… $+1$	… $+2$	… $+3$

⋮

Relaxation data for subshell N_S, transition $NT(N_S)$ (if present):

$Designator(1)$	$Designator(2)$	$Energy$	$Probability$
$JXS(18) + OFF_{rel}(N_S) + 4 \cdot (NT(N_S)-1)$	… $+1$	… $+2$	… $+3$

$E_e(1)$ $JXS(19)$	Energies for all electron cross sections (separate common grid).	… $E_e(N_e)$ $JXS(19) + N_e - 1$
$\sigma_{tot}(1)$ $JXS(19) + N_e$	Total electron cross section.	… $\sigma_{tot}(N_e)$ $JXS(19) + 2 \cdot N_e - 1$
$\sigma_{elas}(1)$ $JXS(19) + 2 \cdot N_e$	Electron elastic cross section.	… $\sigma_{elas}(N_e)$ $JXS(19) + 3 \cdot N_e - 1$
$\sigma_{brems}(1)$ $JXS(19) + 3 \cdot N_e$	Bremsstrahlung cross section.	… $\sigma_{brems}(N_e)$ $JXS(19) + 4 \cdot N_e - 1$
$\sigma_{excit}(1)$ $JXS(19) + 4 \cdot N_e$	Electron excitation cross section.	… $\sigma_{excit}(N_e)$ $JXS(19) + 5 \cdot N_e - 1$
$\sigma_{ion}(1)$ $JXS(19) + 5 \cdot N_e$	Electroionization cross section (total).	… $\sigma_{ion}(N_e)$ $JXS(19) + 6 \cdot N_e - 1$
$\sigma_{ion}^{1}(1)$ $JXS(19) + (5+s) \cdot N_e$	Electroionization cross section for subshell $s = 1$ (K always exists).	… $\sigma_{ion}^{1}(N_e)$ $JXS(19) + (6+s) \cdot N_e - 1$
$\sigma_{ion}^{2}(1)$ $JXS(19) + (5+s) \cdot N_e$	Electroionization cross section for subshell $s = 2$ (if present).	… $\sigma_{ion}^{2}(N_e)$ $JXS(19) + (6+s) \cdot N_e - 1$

⋮

$\sigma_{ion}^{N_S}(1)$ $JXS(19) + (5+N_S) \cdot N_e$	Electroionization cross section for subshell $s = N_S$ (if present).	… $\sigma_{ion}^{N_S}(N_e)$ $JXS(19) + (6+N_S) \cdot N_e - 1$
$E_X(1)$	Energies for tabulating electron	… $E_x(N_{XL})$

$JXS(20)$	excitation energy loss.	$JXS(20)+N_{XL}-1$
$EL_X(1)$ $JXS(20)+N_{XL}$	Average excitation energy loss at each tabulated interaction energy.	… $EL_x(N_{XL})$ $JXS(20)+2\cdot N_{XL}-1$
$E_A(1)$ $JXS(21)$	Electron energies for which there are elastic angular tables.	… $E_A(N_A)$ $JXS(21)+N_A-1$
$L_A(1)$ $JXS(21)+N_A$	Lengths of elastic angular tables.	… $L_A(N_A)$ $JXS(21)+2\cdot N_A-1$
$OFF_A(1)$ $JXS(21)+2\cdot N_A$	Offsets to elastic angular tables. $OFF_A(1)=0$	… $OFF_A(N_A)$ $JXS(21)+3\cdot N_A-1$
$C_{elas}(1,1)$ $JXS(22)$	Tabulated cosines for elastic angular table 1.	… $C_{elas}(L_A(1),1)$ $JXS(22)+L_A(1)-1$
$P_{elas}(1,1)$ $JXS(22)+L_A(1)$	Cumulative probabilities for elastic angular table 1.	… $P_{elas}(L_A(1),1)$ $JXS(22)+2\cdot L_A(1)-1$
$C_{elas}(1,2)$ $JXS(22)+OFF_A(2)$	Tabulated cosines for elastic angular table 2.	… $C_{elas}(L_A(2),2)$ $JXS(22)+OFF_A(2)+L_A(2)-1$
$P_{elas}(1,2)$ $JXS(22)+OFF_A(2)+L_A(2)$	Cumulative probabilities for elastic angular table 2.	… $P_{elas}(L_A(2),2)$ $JXS(22)+OFF_A(2)+2\cdot L_A(2)-1$
⋮		
$C_{elas}(1,N_A)$ $JXS(22)+OFF_A(N_A)$	Tabulated cosines for elastic angular table N_A.	… $C_{elas}(L_A(N_A),N_A)$ $JXS(22)+OFF_A(N_A)+L_A(N_A)-1$
$P_{elas}(1,N_A)$ $JXS(22)+OFF_A(N_A)+L_A(N_A)$	Cumulative probabilities for elastic angular table N_A.	… $P_{elas}(L_A(N_A),N_A)$ $JXS(22)+OFF_A(N_A)+2\cdot L_A(N_A)-1$
$N_i(1)$ $JXS(23)$	Number of electroionization (knock-on) tables by subshell.	… $N_i(N_S)$ $JXS(23)+N_S-1$
$LOC_{info}(1)$ $JXS(23)+N_S$	Location of information about knock-on tables by subshell.	… $LOC_{info}(N_S)$ $JXS(23)+2\cdot N_S-1$

$LOC_{tab}(1)$ $JXS(23) + 2 \cdot N_S$	Location of knock-on tables by subshell.	... $LOC_{tab}(N_S)$ $JXS(23) + 3 \cdot N_S - 1$

Data block for knock-on energies for subshell s. One such block occurs for each $s = 1, \ldots, N_S$

$E_T(1, s)$ $LOC_{info}(s)$	Energies for which knock-on sampling tables are given.	... $E_T(N_i(s), s)$ $LOC_{info}(s) + N_i(s) - 1$
$L_T(1, s)$ $LOC_{info}(s) + N_i(s)$	Lengths of the knock-on sampling tables.	... $L_T(N_i(s), s)$ $LOC_{info}(s) + 2 \cdot N_i(s) - 1$
$OFF_T(1, s)$ $LOC_{info}(s) + 2 \cdot N_i(s)$	Offsets of the knock-on sampling tables.	... $OFF_T(N_i(s), s)$ $LOC_{info}(s) + 3 \cdot N_i(s) - 1$
$E_K^s(1, t)$ $LOC_{tab}(s) + OFF_T(t, s)$	Tabulated knock-on energies for table $t = 1$ for subshell s.	... $E_K^s(L_T(t, s), t)$ $LOC_{tab}(s) + OFF_T(t, s) + L_T(t, s) - 1$
$P_K^s(1, t)$ $LOC_{tab}(s) + OFF_T(t, s) + L_T(t, s)$	Cumulative probabilities of the energies for table $t = 1$ for subshell s.	... $P_K^s(L_T(t, s), t)$ $LOC_{tab}(s) + OFF_T(t, s) + 2 \cdot L_T(t, s) - 1$
⋮		
$E_K^s(1, N_i(s))$ $LOC_{tab}(s) + OFF_T(N_i(s), s)$	Tabulated knock-on energies for table $N_i(s)$ for subshell s.	... $E_K^s(L_T(N_i(s), s), N_i(s))$ $LOC_{tab}(s) + OFF_T(N_i(s), s) + L_T(N_i(s), s) - 1$
$P_K^s(1, N_i(s))$ $LOC_{tab}(s) + OFF_T(N_i(s), s) + L_T(N_i(s), s)$	Cumulative probabilities of the energies for table $N_i(s)$ for subshell s.	... $P_K^s(L_T(N_i(s), s), N_i(s))$ $LOC_{tab}(s) + OFF_T(N_i(s), s) + 2 \cdot L_T(N_i(s), s) - 1$

End of data block(s) for knock-on energies by subshell.

$E_B(1)$ $JXS(24)$	Electron energies for which there are bremsstrahlung energy tables.	... $E_B(N_B)$ $JXS(24) + N_B - 1$
$L_B(1)$ $JXS(24) + N_B$	Lengths of bremsstrahlung energy tables.	... $L_B(N_B)$ $JXS(24) + 2 \cdot N_B - 1$

$OFF_B(1)$ $JXS(24)+2\cdot N_B$	Offsets to bremsstrahlung tables. $OFF_B(1)=0$	... $OFF_B(N_B)$ $JXS(24)+3\cdot N_B-1$
$E_{brems}(1,1)$ $JXS(25)$	Tabulated energies for bremsstrahlung table 1.	... $E_{brems}(L_B(1),1)$ $JXS(25)+L_B(1)-1$
$P_{brems}(1,1)$ $JXS(25)+L_B(1)$	Cumulative probabilities for bremsstrahlung table 1.	... $P_{brems}(L_B(1),1)$ $JXS(25)+2\cdot L_B(1)-1$
$E_{brems}(1,2)$ $JXS(25)+OFF_B(2)$	Tabulated energies for bremsstrahlung table 2.	... $E_{brems}(L_B(2),2)$ $JXS(25)+OFF_B(2)+L_B(2)-1$
$P_{brems}(1,2)$ $JXS(25)+OFF_B(2)+L_B(2)$	Cumulative probabilities for bremsstrahlung table 2.	... $P_{brems}(L_B(2),2)$ $JXS(25)+OFF_B(2)+2\cdot L_B(2)-1$
⋮		
$E_{brems}(1,N_B)$ $JXS(25)+OFF_B(N_B)$	Tabulated energies for bremsstrahlung table N_B.	... $E_{brems}(L_B(N_B),N_B)$ $JXS(25)+OFF_B(N_B)+L_B(N_B)-1$
$P_{brems}(1,N_B)$ $JXS(25)+OFF_B(N_B)+L_B(N_B)$	Cumulative probabilities for brems. table N_B.	... $P_{brems}(L_B(N_B),N_B)$ $JXS(25)+OFF_B(N_B)+2\cdot L_B(N_B)-1$
$E_{BL}(1)$ $JXS(26)$	Energies for tabulating average bremsstrahlung energy loss.	... $E_{BL}(N_{BL})$ $JXS(26)+N_{BL}-1$
$ER_{BL}(1)$ $JXS(26)+N_{BL}$	Kinetic energy remaining with the electron after average loss to bremsstrahlung.	... $ER_{BL}(N_{BL})$ $JXS(26)+2\cdot N_{BL}-1$

III. SUMMARY

We have presented a full description of the format and contents of electron/photon/relaxation data tables contained in the new ACE-format library **eprdata12**. This documentation is complete and consistent with the data as released with the first production release of MCNP6. We hope that MCNP users, code developers, and data specialists will find this to be a useful guide to the details of current electron/photon/relaxation data used in MCNP6.

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