LA-UR-03-0787

Approved for public release; distribution is unlimited.

Title: Photoatomic Data Library MCPLIB03: An Update to MCPLIB02 Containing Compton Profiles for Doppler Broadening of Incoherent Scattering

Los Alamos National Laboratory memorandum X-5:MCW-02-110

Author(s): Morgan C White

Submitted to: Electronic Documentation Available at www-xdiv.lanl.gov/PROJECTS/DATA/nuclear/avdoc.htm

Los Alamos
NATIONAL LABORATORY
memorandum
Applied Physics Division
Diagnostics Applications Group X-5
Phone (505) 667-8747 Fax (505) 665-3046

To/MS: Distribution
From/MS: Morgan C White, X-5, MS F663
Phone/Email: 5-3684 / morgan@lanl.gov
Symbol: X-5:MCW-02-110(U)
Date: December 19, 2002

SUBJECT: Photoatomic Data Library MCPLIB03: An Update to MCPLIB02 Containing Compton Profiles for Doppler Broadening of Incoherent Scattering

Summary

This memo announces the availability of MCPLIB03, a new photoatomic data library, for use with the MCNP transport code. This library contains data for elements Z equal 1 to 94 accessed using ZAIDs[1] like ZZ000.03p where ZZ is the appropriate atomic number. This library is an extension of the MCPLIB02 [1] library. MCPLIB02 and MCPLIB03 contain identical cross-section, fluorescence and form factor data. MCPLIB03 has been extended to include the Compton profile data of Biggs et al. [2] suitable for calculating the Doppler broadening of the energy for Compton scattered photons. The coding necessary to use such data has been added to MCNP5 [3,4]. The Doppler broadening energy sampling algorithm and the extensions to the photoatomic data storage format are discussed in references [5,6]. This library will be available in the usual locations for LANL users and available as part of the RSICC DLC-220 MCNP data distribution for external users.

A Brief History Of The Photoatomic Data

Until this year, MCNP users have had "two" (in quotes to note their close relation) photoatomic data libraries from which to choose. It is worth reviewing their lineage so as to provide the end user a more comprehensive understanding of exactly what data they are using. Note that MCPLIB and MCPLIB02 contain data for elements Z equal 1 to 94 for the coherent, incoherent, total photoelectric and total pair production cross sections; for the coherent form factor; for the incoherent scattering function; and, for simple fluorescence parameters. Interested readers may want to consult references [7,8] that describe the origins of the MCNP photon transport algorithms.

Lineage of MCPLIB

MCPLIB [9] has been available since 1982 and uses the ID '01p'. It contains coherent, incoherent, total photoelectric and total pair production cross-section data as well as incoherent

[1] A ZAID is the unique identifier for a data table. The ID portion of this is a unique integer library number and a character table type, e.g. '03p' indicates a photoatomic data table belonging to the MCPLIB03 library.

scattering function, coherent form factor, and fluorescence data for elements with atomic number (Z) equal 1-94.

The cross section data for elements Z equal 1-83, 86, 90, 92 and 94 in this library were originally produced in 1969 by evaluators at the Lawrence Livermore National Library (probably one of the first versions of the Evaluated Photon Data Library EPDL) and revised over the following years. The data were reviewed by Hubbell at NIST and first made available through RSICC as package DLC-007 version C. Form factor and scattering function data were added in 1975 along with updated cross section information. This revision was released through RSICC as DLC-007 version E [10]; reviewed by the Cross Section Evaluation Working Group (the governing body for the U.S. ENDF/B library) and released through the National Nuclear Data Center as ENDF/B-IV [11]; and documented in the Hubbell et al. article [12]. There was an additional update after this point but that update was not used by MCPLIB.

The data for the missing elements – Z equal 84, 85, 87, 88, 89 and 93 – were taken from the previous MCP library. These data derive from evaluations done by Storm and Israel. Their first data compilation was reported in 1967 [13]. These data were later revised and published [14] with an electronic version made available through RSICC as package DLC-015 [15]. This library contained cross section data for the energy range 1 keV to 100 MeV for elements Z equal 1 to 100 but did not include form factor or scattering function data. The cross section data for elements Z equal 84, 85, 87-89 and 93 on MCPLIB may be traced to this updated Storm and Israel library although the MCPLIB tables contain tabulations for the energy range 1 keV to 15 MeV, i.e. they do not contain the data available up to 100 MeV. At the time this memorandum was written, we still cannot trace the lineage of the form factor or scattering function data for these elements. It is worth noting that Hubbell reviewed the DLC-7e and DLC-15 libraries in the early 1970's and found them in substantial agreement.

Lineage of MCPLIB02

MCPLIB02 [1] has been available since 1993. It is an extension of the MCPLIB library such that cross section data are available for elements Z equal 1 to 94 in the energy range 1 keV to 100 GeV. MCPLIB and MCPLIB02 contain identical cross section data below 10 MeV; the form factor, scattering function and fluorescence data are also unchanged. Above the highest energy for each element in the MCPLIB library, the cross section data are taken directly from the EPDL89 library [16]. A smooth transition is made between 10 MeV and (1) 100 MeV for elements Z equal 1-83, 86, 90, 92 and 94, and (2) 15 MeV for elements Z equal 84, 85, 87-89 and 93.

Lineage of the Fluorescence Data For MCPLIB and MCPLIB02

The fluorescence algorithm still in use today was taken from the MCP code. This algorithm is well documented by Everett and Cashwell [17] and every library to date (MCPLIB, MCPLIB02 and MCPLIB03) has used the fluorescence data as listed in Table 1 therein. The algorithm accounts for fluorescence in an approximate manner as described below. The reason for the longevity of this data has been the difficulty in obtaining a complete set of data from which to derive the necessary parameters. A complete data set requires probabilities of ejecting electrons

from each shell and probabilities for each possible radiative (i.e. x-rays) or non-radiative (i.e. auger electron) transfer resulting from any electron vacancy. The first such complete data set known to this author was not produced until very recently (1997) [18]. Everett and Cashwell derived their parameters from a widely dispersed set of data and were forced to make many assumptions [17]. It is worth noting that the parameters produced are consistent (i.e. the fluorescence energy is consistent with the photoelectric edge values) with the Storm and Israel 1970 cross-section data [14]. Truly keen observations may note that the current algorithm for second fluorescence (since version 2C) differs from the original algorithm. This difference derives from a bug fix [19,20,21,22] to correct the algorithm; specifically equation (6) in reference [17] should read $Y_{L3} = Y_{L2} = Y_{L1} = Y_L$.

The fluorescence algorithm and data is a crude approximation of the true relaxation cascade. As designed it emits "fluorescence" x-rays with combined probabilities and weighted average energies. These might represent a real line – with the appropriate transition probability and energy – or it might represent an averaged line – with the combined transition probability of several lines and their weighted average energy. No lines are ever present for elements with Z less than 12 as all emission are less than 1 keV (the current MCNP photon and electron energy cutoff). Similarly, no transitions to L shell vacancies are considered for Z less than 37 as these emissions are less than 1 keV. Double fluorescence is only considered for elements with Z greater than 36 as it requires that the primary fluorescence is a K transition thus leaving a vacancy for a second transition to the L shell. Table 1 below indicates by elemental range what "lines" are included in this data.

Table 1. Fluorescence "lines" given in the data libraries as a function of element.

Elements (Z equal to)	K (ave. of L2-K and L3-K)	K1 (L3-K)	K2 (L2-K)	K1 (ave. of all M-K)	K2 (ave. of all N-K)	L (ave. of all trans. to L)
1-11						
12-19	*					
20-30		*	*	*		
31-36		*	*	*	*	
37-94		*	*	*	*	*

Comments about Photon Heating Values

The photon heating values are given in units of MeV per collision and typically used as a reaction rate multiplier to arrive at energy deposition rates in a material. These average heating values assume instantaneous local deposition of all secondary electron energy. Specifically, the average heating value is calculated according to Equation 1 where E_i is the incident photon energy; $\overline{E}_{p,x}$ is the average secondary photon energy where x is 'inc' for incoherent scattering, 'pe' for photoelectric events and 'pp' for pair production events; and, the are the corresponding cross-section values. The average energy for incoherent scattered photons accounts for the form factor effect on the scattered distribution. The average energy for fluorescence x-rays is the

average of the possible x-rays. The average energy for pair production is 2*0.511 MeV (accounting for the annihilation photons from a positron at rest; MCNP does not account for in-flight annihilation).

$$H(E_i) = \frac{\sigma_{inc}(E_i) \cdot \left(E_i - \bar{E}_{p,inc}(E_i)\right) + \sigma_{pe}(E_i) \cdot \left(E_i - \bar{E}_{p,pe}(E_i)\right) + \sigma_{pp}(E_i) \cdot \left(E_i - \bar{E}_{p,pp}(E_i)\right)}{\sigma_T(E_i)} \quad \text{Eq. 1}$$

Known Limitations of the MCPLIB and MCPLIB02 Data

The expert MCNP user should be aware of several limitations in the MCNP photon algorithms and data. They are reiterated here (in no particular order) to remind us all. First, for incident photon energies less than 10 MeV the cross-section, form factor, scattering function and fluorescence data contained in both MCPLIB and MCPLIB02 date back to photon evaluations performed in the early 1970's. Hence, in this critical energy range (1 keV to 10 MeV) the data is outdated (though usually within a few percent of the modern value). Many advances have been made in our understanding of this regime.

Second, at all energies these data are given on a fairly course energy grid and log-log interpolation is used between values. Given a tally of the uncollided photons using a fine bin structure, a plot using linear axes will show "scalloping"; this is an artifact of the energy grid and interpolation scheme imprinting on the tally,

Third, the photon heating numbers were designed for photon only transport problems and are meant for "engineering"-type solutions (i.e. somewhat rough approximations). The assumption of instantaneous local deposition of all secondary electron energy can often be far from truth. As the incident photon energy increases, these secondary electrons can travel very far; bremsstrahlung reactions extend their reach (and the true location of the energy deposition) even further. It is also worth noting that if electron transport or the thick-target bremsstrahlung option are used, the resulting tertiary (photon-electron-photon) photons are not counted in a heating tally (to prevent double-counting). Given these caveats, the photon heating numbers perform remarkably well and are able to give reasonable estimates in many situations. However, if accurate energy deposition is desired, an F8 tally is still the best method.

Fourth, the fluorescence data in these libraries contain many assumptions. Besides the assumptions outlined above (Lineage of the Fluorescence Data), note that the non-radiative transitions (auger electron emissions) were once entirely ignored and are now approximated with one emission based on the (uncorrelated) electron data. Note one of the original author's (Everett) quote in reference [20]: "The [library] constants used in the [fluorescence] photon code involve so many wild guesses that it doesn't matter much what is done about secondary fluorescence. I really think the whole thing should be revamped – I hope it isn't used much. Surely its results should not be taken very seriously." At the time these data were produced, much of the knowledge necessary to produce them was just becoming understood and measured. It is remarkable how well these data have done, all things considered. Certainly they have lived

up to their author's intent and been more than adequate for producing roughly the right energy re-emission. That said, one should be skeptical (if not disbelieving) of calculations of x-ray lines and energy deposition in very small regions far way from electron equilibrium.

MCPLIB03 / Compton Profile Data

MCPLIB03 is another extension of this ongoing photoatomic data library. The cross section, form factor, scattering function and fluorescence data are identical to MCPLIB02. The only difference is the addition of Compton profile data for use in calculating the Doppler energy broadening for incoherent scattered photons.

The raw Compton profile data from which the data in MCPLIB03 derive are identical[2] to Table I of reference [2]. According to reference [2] equation 10 (reproduced here as equation 2 where J_{nl} is the Compton profile for the shell with quantum number n and l and p_z is the electron momentum), the profile for each shell should integrate to one-half (remembering that half the distribution is given as it is symmetric). No guidance is given in the paper on the interpolation scheme to be used between points. Using linear-linear interpolation, each of the profiles meets this criterion to within 10%. The agreement is worse for higher Z and inner shells. For the most part, it is near 1 to 2% except at high Z. (Other interpolation schemes were also considered. While log-linear interpolation might have been used, as the integral was slightly more consistent, inverting the log-linear integration in order to sample p_z would have required considerably more effort.)

$$2\int_0^{\infty} J_{nl}(p_z)\,dp_z = 1 \qquad \text{Equation 2}$$

The end goal for using these data in a calculation is to sample a shell and then sample a momentum value (p_z) based on the profile for that shell. The photoatomic format has been extended [6] in order to hold these new data. The electron momentum is used to calculate the broadening of the energy due to the motion of the bound electron during a Compton scattering event (see reference [5] for the MCNP5 implementation details or reference [23] for a different perspective). In order to sample the momentum, the raw profile data from [2] have been normalized according to Equation 3 to provide the standard value, PDF, CDF type distribution[3] commonly used throughout MCNP (see equation 4).

---

[2] To be fully honest (always read the fine print), Avneet Sood obtained and used an electron copy of these data while working on his Ph.D. thesis in this subject at NC State. His electronic version has been "spot" checked against the reference table and no inconsistencies have been discovered.

[3] MCNP stores many sampling tables using a scheme with the Sampled Value, Probability Distribution Function (PDF) and Cumulative Distribution Function (CDF). A random number (0,1) chooses a bin based on the CDF and a sampled value is selected based on interpolation within the bin using the appropriate PDF values.

$$\int_0^{100} J_i(p_z)\,dp_z = 1 \qquad \text{Equation 3}$$

$$\square = \int_0^{p_z} J_i(Q)\,dQ \qquad \text{Equation 4}$$

The other required set of data is the probability that the scattering event happens with an electron from shell *i*. There were no data (nor advice) offered for selecting this shell. As no other solution presented itself, the (almost certainly incorrect) assumption was made that the probability of interacting with an electron in a given shell is equal to the number of electrons in that shell divided by the total number of electrons. This obviously ignores any screening effects. This assumption should be revisited (and corrected).

Last Words

The reason for creating the MCPLIB03 data library was to add the Compton profile data described herein to an existing photoatomic library for the purposes of comparison to previous calculations. These data are necessary to increase the fidelity with which the underlying physics are represented. The source and processing of these new data are documented for traceability.

The lineage of the photoatomic data in MCPLIB03 has been given in great detail. As it is an extension of the MCPLIB02 library which is itself an extension of the MCPLIB library, these libraries have also been described. This historical tour is provided to the user in order to fully document the origins and lineage of these data libraries. In addition to source documentation, some of the limitations and inconsistencies in the libraries are also documented.

As always, the user may use the plot features of MCNP to examine these new data or compare them to previous data. Note that the 'printpts' is a useful tool to dump the data into a two column format suitable for importing into other graphing programs.

While the MCPLIB03 library is only an extension to add the Compton profile data to an existing library, a truly new photoatomic library is also being released at this time. MCPLIB04 [24] is being released with data for elements Z equal 1 to 100 from the ENDF/B-VI release 8 evaluated data library. It is therefore recommended that MCPLIB03 only be used for comparison purposes. MCPLIB04 will become the recommended library at this time.

References

[1] H. Grady Hughes. "Information on the MCPLIB02 Photon Library." Los Alamos National Laboratory memorandum X-6:HGH-93-77 (January 28, 1993).

[2] F. Biggs, L. B. Mendelsohn and J. B. Mann. "Hartree-Fock Compton Profiles For The Elements." Atomic Data and Nuclear Data Tables, Vol. 16, pp. 210-309 (1975).

[3] "MCNP5 (Version MCNP5_RSICC/1)" Los Alamos National Laboratory Computer Code LA-CC-02-083 (December 2002).

[4] Forrest B. Brown. "MCNP5 (Versions MCNP5_LANL/1 and MCNP5_RSICC/1)" Los Alamos National Laboratory memorandum X-5:FBB-02-01 (December 11, 2002).

[5] Avneet Sood. "Doppler Energy Broadening for Incoherent Scattering in MCNP: Part I." Los Alamos National Laboratory Research Note X-5:AS-02-16 (July 31, 2002).

[6] Avneet Sood and Morgan C White. "Doppler Energy Broadening for Incoherent Scattering in MCNP: Part II." Los Alamos National Laboratory Research Note X-5:AS-02-17 (July 31, 2002).

[7] L. L. Carter and E. D. Cashwell. "Particle-Transport Simulation with the Monte Carlo Method." ERDA Critical Review Series TID-26607, National Technical Information Service (October 1975).

[8] E. D. Cashwell, J. R. Neergaard, C. J. Everett, R. G. Schrandt, W. M. Taylor and G. D. Turner. "Monte Carlo Photon Codes: MCG and MCP." Los Alamos National Laboratory report LA-5157-MS (March 1973).

[9] Robert C. Little. "New Photon Library From ENDF Data." Los Alamos National Laboratory memorandum X-6:RCL-82-2/26 (February 26, 1982).

[10] "RSIC Data Library DLC-007; HPICE: Evaluated Photon Interaction Library, ENDF/B File 23 Format." Radiation Safety Information Computational Center package DLC-007e, Oak Ridge National Laboratory (July 1975).

[11] Cross Section Evaluation Working Group. "ENDF/B-IV Summary Documentation." Report ENDF-201 rev 1975, National Nuclear Data Center, Brookhaven National Laboratory (1975).

[12] J. H. Hubbell, W. J. Veigele, E. A. Briggs, R. T. Brown, D. T. Cromer and R. J. Howerton. "Atomic Form Factors, Incoherent Scattering Functions and Photon Scattering Cross Sections." Journal of Physical and Chemical Reference Data, Vol. 4, Issue 3, pp. 471-538 (1975).

[13] Ellery Storm and Harvey I. Israel. "Photon Cross Sections from 0.001 to 100 MeV for Elements 1 through 100." Los Alamos National Laboratory report LA-2753 (June 1967).

[14] Ellery Storm and Harvey I. Israel. "Photon Cross Sections from 1 keV to 100 MeV for Elements Z = 1 to Z = 100." Nuclear Data Tables Section A, Vol. 7, pp. 565-581 (June 1970).

[15] "RSIC Data Library DLC-015; STORM-ISRAEL: Evaluated Photon Interaction Library, ENDF/B File 23 Format." Radiation Safety Information Computational Center package DLC-015, Oak Ridge National Laboratory (January 1971).

[16] D. E. Cullen, M. H. Chen, J. H. Hubbell, S. T. Perkins, E. F. Plechaty, J. A. Rathkopf and J. H. Scofield. "Tables and Graphs of Photon-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Photon Data Library (EPDL)." Lawrence Livermore National Laboratory report UCRL-50400, Vol. 6 (October 31, 1989).

[17] C. J. Everett and E. D. Cashwell. "MCP Code Fluorescence-Routine Revision." Los Alamos National Laboratory report LA-5240-MS (May 1973).

[18] D. E. Cullen, J. H. Hubbell and Lynn Kissel. "EPDL97: The Evaluated Photon Data Library, '97 Version." Lawrence Livermore National Laboratory report UCRL-50400, Vol. 6, Revision 5 (September 19, 1997).

[19] Joe Devaney. "Review of the Fluorescence Section of MCNP." Los Alamos National Laboratory memorandum X-6:JD-82-1/15 (January 15, 1982).

[20] Joe Devaney. "Proposed Changes To The Fluorescence Part Of MCNP (Detailed Photon Physics – MCP)." Los Alamos National Laboratory memorandum X-6:JD-82-1/18 (January 18, 1982).

[21] Buck Thompson. "Everett's Comments on Fluorescence." Los Alamos National Laboratory memorandum X-6:WLT-82-2/17 (February 17, 1982).

[22] Joe Devaney. "Second Review of Fluorescence." Los Alamos National Laboratory memorandum X-6:JD-82-7/12 (July 12, 1982).

[23] Y. Namito, S. Ban and H. Hirayama. "Implementation of the Doppler broadening of a Compton-scattered photon into the EGS4 code." Nuclear Instruments and Methods in Physics Research Section A, Vol. 349, pp. 489-494 (1994).

[24] Morgan C White. "Photoatomic Data Library MCPLIB04: A New Photoatomic Library Based On Data From ENDF/B-VI Release 8." Los Alamos National Laboratory memorandum X-5:MCW-02-111 (December 19, 2002).