LA-UR-03-1019

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Title: Photoatomic Data Library MCPLIB04: A New Photoatomic Library Based On Data from ENDF/B-VI Release 8

Author(s): Morgan C. White,
Los Alamos National Laboratory, Los Alamos, NM

Submitted to: Documentation for the MCNP user community via the web.

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Form 836 (8/00)

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-02-111(U)
Date: December 19, 2002
Revised February 7, 2003

SUBJECT: Photoatomic Data Library MCPLIB04: A New Photoatomic Library Based On Data from ENDF/B-VI Release 8

Summary

This memo announces the availability of MCPLIB04, a new photoatomic data library for use with the MCNP transport code. The core of this library is a completely new set of data taken from ENDF/B-VI release 8 [1] including cross section, form factor, scattering function and fluorescence data. These data are derived from EPDL97; for detailed descriptions, please see the original reference [2]. Tables are included in this library for elements Z equal 1 to 100 (finally providing tables for elements Z equal 95 to 100) in the energy range 1 keV to 100 GeV. These tables are significantly denser (i.e. they contain more energy points in the tabulation) and therefore more accurately represent the cross-section data than the earlier photon libraries. In addition to these core data, MCPLIB04 has been extended to include the Compton profile data of Biggs et al. [3] 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 [4,5]. The Doppler broadening energy sampling algorithm and the extensions to the photoatomic data storage format are discussed in references [6,7]. This library will be available in the usual locations for LANL users[1] and available as part of the RSICC DLC-220 MCNP data distribution for external users. The MCPLIB04 library uses the library ID '04p'; individual ZAIDs range from 1000.04p through 100000.04p.

A Brief History Of The Previous Photoatomic Data

Until this year, MCNP users have had "two" (in quotes to note their close relation) photoatomic data libraries from which to choose. MCPLIB [8] and MCPLIB02 [9] 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. In both libraries, the data in the energy range less than 10 MeV derive from compilations by Storm and Israel [10] or Hubbell et al. [11] dating back to the early 1970's. Many advances have been made in our understanding of this key energy range since that time. A more detailed discussion on the origins of these libraries is given in reference [12]. Reference

[1] See http://laurel.lanl.gov/PROJECTS/DATA/nuclear/doc/datapath.html

[12] also documents MCPLIB03 that is yet another extension to the earlier MCPLIB libraries to include the Compton profile data [3]. Readers interested in the origins of the MCNP photon transport algorithms may find references [13,14] useful.

Overview of MCPLIB04 Data

The MCPLIB04 library contains photoatomic data tables for elements Z equal 1 to 100. Each table contains coherent, incoherent, total photoelectric and total pair production cross-section data for the incident photon energy range 1 keV to 100 GeV. Also included are coherent form factor and incoherent scattering function data given on the traditional MCNP fixed grids and atomic relaxation data given in the traditional fluorescence data format (for the grid specifications and fluorescence data format see Appendix F, Section VII [15]). These data were processed using NJOY 99.82 [16,17,18] as described below. In addition to these core data, Compton profile data are included for use in calculating the Doppler energy broadening for scattered photons from Compton events. Various aspects of these data will be discussed below.

Data Sources

The evaluated data from which the MCPLIB04 cross-section, form factor, scattering function and fluorescence data derive are available as part of the ENDF/B-VI release 8 [1] data library. The data are publicly available through the US National Nuclear Data Center web site. These evaluations are originally from the Lawrence Livermore National Laboratory EPDL/EADL data libraries. References [2,19] describe the history of the LLNL library including the experimental data and theoretical models from which these evaluated data derive.

The Compton profile data used in MCPLIB04 are derived from the Biggs et al. article [3]. These data were obtained (third-hand) in electronic format and spot checked against the numbers in the original article. Note that the Compton profile data do not derive from an evaluated data source, e.g. the ENDF/B library. Specifically, this is a warning that these data have not undergone the extensive QA peer-reviews to which an evaluated data source is subject.

NJOY Processing

NJOY99 has been modified [18] to allow it to process ENDF-6 format [20] photoatomic and atomic relaxation evaluated data into the ACE continuous-energy photoatomic format [15]. NJOY99 has from its inception been able to process cross section, form factor and scattering function data into the ACE format. Only recently have atomic relaxation data – necessary for the fluorescence data calculation – been available as part of the ENDF/B library. Several NJOY99 updates are particularly noteworthy for processing these new data. Update 69 contains the original coding to handle the fluorescence data processing; update 80 fixed a bug to correctly handle discontinuities at photoelectric edges; and, update 82 updated the coding to calculate photon heating values. The final version of the MCPLIB04 library was produced on 02/07/03 using NJOY99.82. It is worth discussing some of the processing steps in order to better understand the library and its limitations.

Cross-Section, Form Factor and Scattering Function Data

The ACE photoatomic format stores the coherent, incoherent, total photoelectric and total pair production cross sections. During processing, the union of all necessary energy grids is used to ensure that no accuracy is lost in representing these data. All cross section values (and energies) are stored as the log of the value in order to facilitate log-log interpolation between the values. The coherent and incoherent cross-section data inherently include the effects of the form factor and scattering function data (e.g. the incoherent cross section matches the integrated Klein-Nishina cross section as modified by the scattering function). Of significant note, the form factor and scattering function data are stored on a fixed grid (see [15] Appendix F page F-39); this fixed grid may not extend far enough in momentum space for the data to asymptote. The photoelectric cross section is the total of all sub-shells; selection of the sub-shell for a given collision is made on the basis of the "parallel assumption" which assumes that the fraction given by the jump at a sub-shell edge remains constant over all energy. The pair production cross section is the total of the pair and triplet cross sections although all collisions are treated as pair production events.

The MCPLIB04 (ENDF/B-VI.8) data represent a significant update to the photon cross section data available for use in MCNP. Most significantly, they contain the benefit of almost three decades of experimental data and theoretical model development past the data available in previous MCNP libraries. Also of note, they are given on a much finer energy grid and thus their use in a transport problem is less subject to imprinting of the log-log interpolation scheme.

Understanding the Legacy Fluorescence Data Format

The fluorescence algorithm still in use today was taken from the MCP code. This algorithm is well documented by Everett and Cashwell [21] and every previous library to date (MCPLIB, MCPLIB02 and MCPLIB03) has used the fluorescence data as listed in Table 1 therein. (A slight modification to the original algorithm is discussed in [22-25].) 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 MCPLIB04 library makes use of such a data set [1,2].

The MCNP 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 photon and electron energy cutoff). Similarly, no transitions to L shell vacancies are considered for Z less than 31 as these emissions are less than 1 keV. Double fluorescence is only considered for elements with Z greater than 30 as it requires that the primary fluorescence is a Kα transition thus leaving a vacancy for a

transition to the L shell. Table 1 below indicates by elemental range what "lines" are included in the MCPLIB04 data.

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

Elements (Z equal to)	Kα	Kα1 (L3-K)	Kα2 (L2-K)	Kβ1	Kβ2	L (ave. of all trans. to L)
1-11						
12-19	(a)					
20-30		(b)	(c)	(d)		
31-36		(b)	(c)	(d)		(g)
37-100		(b)	(c)	(e)	(f)	(g)

It is worth noting what data NJOY99.82 uses to create these various "lines" as they are slightly different from the previous fluorescence data. Elements Z equal 12 to 19 contain only one "line" (a); this is the average of all possible radiative transitions to the K shell. All elements Z greater than or equal 20 contain the two real lines (b&c) Kα1 – L3 to K – and Kα2 – L2 to K. These key lines are important for their use as elemental identifiers in spectrometry. The line (d) for elements Z equal 20 to 36 is the average of all other possible radiative transitions to the K-shell. For elements Z greater than or equal to 37, line (e) is the average of all radiative transitions from the M-shell to the K-shell and line (f) all remaining transitions to the K-shell. The remaining line (g) for elements Z greater than or equal 31 is the average of all other possible radiative transitions to the L-shells (collectively).

Besides the assumptions inherent in the description above, one further comment is needed: the non-radiative transitions (auger electron emissions) were once entirely ignored and are now approximated with one emission based on the (uncorrelated) electron data.

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, $E_{p,x}$ is the average secondary photon energy for process *x* and the σ_x 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).

$$H = \frac{\sigma_{inc}\left(E_i - \overline{E}_{p,inc}\right) + \sigma_{pe}\left(E_i - \overline{E}_{p,pe}\right) + \sigma_{pp}\left(E_i - \overline{E}_{p,pp}\right)}{\sigma_T} \qquad \text{Equation (1)}$$

Note that 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. Note that if electron transport or the thick-target bremsstrahlung option are used, the resulting tertiary (photon-electron-photon) photons are explicitly excluded from contributing to the heating tallies. Given the caveats described above, 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.

MCPLIB04 / Compton Profile Data

In addition to the core data, MCPLIB04 includes 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 MCPLIB04 derive are identical[2] to Table I of reference [3]. According to reference [3] equation 10 (reproduced here as equation 2), 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 the electron momentum 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 [7] 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 [6] for the MCNP5 implementation details or reference [26] for a different perspective). In order to sample the momentum, the raw profile data from [3] have been

[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.

normalized according to Equation 3 to provide the standard value, PDF, CDF type distribution[3] commonly used throughout MCNP (see equation 4).

$$\int_0^{100} J_i(Q)dQ = 1 \qquad \text{Equation 3}$$

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

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). Note that the Compton profile data on MCPLIB04 are identical to those on MCPLIB03 [12].

Last Words

The lineage of the photoatomic data in MCPLIB04 (ID plib = '04p') has been given in great detail. The core of this library – derived from the ENDF/B-VI.8 evaluated data set – represents a significant new set of photoatomic data for use in MCNP photon calculations. The Compton profile data also included in this library are documented along with their processing for final use in MCNP. In addition to various descriptions of the library, some of the limitations inherent in the ACE photoatomic format and MCNP algorithms are also documented herein.

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