TABLES AND GRAPHS OF PHOTON- INTERACTION CROSS SECTIONS FROM 0.1 keV TO 100 MeV DERIVED FROM THE LLL EVALUATED- NUCLEAR-DATA LIBRARY

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MASTER

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FOREWORD

The UCRL-50400 series describes an integrated and computer-oriented system for the production and application of neutronics and photonics calculational constants.

The system must supply reliable up-to-date data, select specific types of data on request, provide output in a variety of forms (ultimately in the form of input to other computer codes), and function rapidly and efficiently. The system has now been developed to a point where we are achieving these goals.

The UCRL-50400 series, *An Integrated System for Production of Neutronics and Photonics Calculational Constants*, comprises the following volumes:

- Vol. 1, Part A, Rev. 3, *ECSIL: A System for Storage, Retrieval, and Display of Experimental Neutron Data*, September 1976.
- Vol. 1, Part B, *Program ECSX4 (Version 78-1): Conversion of Experimentally Measured Cross Section Data from the Four-Center-Exchange (X-4) Format to the Livermore ECSIL Format*, 1979.
- Vol. 2, Rev. 2, *A Bibliography of the Experimental Data of Neutron-Induced Interactions*, July 1976.
- Vol. 3, Rev. 2, *An Index of the Experimental Data of Neutron-Induced Interactions*, July 1976.
- Vol. 4, *Evaluated Nuclear Cross-Section Library*, April 1971.
- Vol. 5, Part A, Rev. 1, *CLYDE: A Code for the Production of Calculational Constants from Nuclear Data*, September 1975.
- Vol. 5, Part B, Rev. 1, *Relativistic Transformations between Center-of-Mass and Laboratory Systems for Two-Body Nuclear Reactions*, April 1978.
- Vol. 6, Rev. 2, *Tables and Graphs of Photon-Interaction Cross Sections from 1 keV to 100 MeV*, December 1978.
- Vol. 7, Part A, Rev. 1, *Major Neutron-Induced Interactions ($Z \leq 55$): Graphical, Experimental Data*, July 1976.
- Vol. 7, Part B, Rev. 1, *Major Neutron-Induced Interactions ($Z > 55$): Graphical, Experimental Data*, July 1976.
- Vol. 8, Part A, Rev. 1, *Supplemental Neutron-Induced Interactions ($Z \leq 35$): Graphical, Experimental Data*, July 1976.
- Vol. 8, Part B, Rev. 1, *Supplemental Neutron-Induced Interactions ($Z > 35$): Graphical, Experimental Data*, July 1976.
- Vol. 9, *Thresholds of Nuclear Reactions Induced by Neutrons, Photons, Deuterons, Tritons, and Alpha Particles*, September 1970.
- Vol. 10, Rev. 1, *Tabulated Experimental Data for Neutron-Induced Interactions*, July 1976.
- Vol. 11, *Experimental Data, Indexes, and Techniques of Obtaining a Selected Set of Neutron Resonance Parameters*, May 1972.
- Vol. 12, *An Atlas of Resolved Neutron Resonance Parameters*, July 1972.
- Vol. 13, *An Atlas of Unresolved Neutron Resonance Parameters*, September 1972.
- Vol. 14, *TARTNP: A Coupled Neutron-Photon Monte Carlo Transport Code*, February 1976.
- Vol. 15, Part A, *The LLL Evaluated-Nuclear-Data Library (ENDL): Evaluation Techniques, Reaction Index, and Descriptions of Individual Evaluations*, September 1975.
- Vol. 15, Part B, Rev. 1, *The LLL Evaluated-Nuclear-Data Library (ENDL): Graphs of Cross Sections from the Library*, October 1978.
- Vol. 15, Part C, *The LLL Evaluated-Nuclear-Data Library (ENDL): Translation of ENDL Neutron-Induced Interaction Data into the ENDF/B Format*, April 1976.
- Vol. 15, Part D, Rev. 1, *The LLL Evaluated-Nuclear-Data Library (ENDL): Descriptions of Individual Evaluations for $Z = 0-98$* , May 1978.
- Vol. 16, Rev. 2, *Tabular and Graphical Presentation of 175 Neutron-Group Constants Derived from the LLL Evaluated-Nuclear-Data Library (ENDL)*, October 1978.

- Vol. 17, Part A, *Program LINEAR (Version 77-1): Linearize Data in the Evaluated-Nuclear-Data File/Version B (ENDF/B) Format*, January 1977.
- Vol. 17, Part B, *Program SIGMA1 (Version 77-1): Doppler Broaden Evaluated Cross Sections in the Evaluated-Nuclear-Data File/Version B (ENDF/B) Format*, January 1977.
- Vol. 18, *ACTL: Evaluated Neutron Activation Cross-Section Library*, 1979.
- Vol. 19, *Neutron-Induced Angular and Energy Distributions: Graphical Experimental Data*, April 1977.
- Vol. 20, *Bonderenko Self-Shielded Cross Sections and Multiband Parameters Derived from the LLL Evaluated-Nuclear-Data Library (ENDL)*, July 1978.

CONTENTS

Foreword	iii
Abstract	vi
1978 Edition	vi
Sources of Evaluated Cross-Section Data	vi
Form Factors, Coherent Cross Sections, and Incoherent Cross Sections	vi
Pair-Production Cross Sections	vi
Photoelectric Cross Sections	vii
Fluorescence Data	vii
Procedures Used to Derive Data	viii
Total Mean Free Path	viii
Energy Deposition	viii
Incoherent Energy Deposition	ix
Coherent Energy Deposition	ix
Pair-Production Energy Deposition	ix
Photoelectric Energy Deposition	x
Bremsstrahlung Energy	xi
Table and Graph Conventions	xi
Production of the Volume	xi
References	xi
Tables and Graphs	I

TABLES AND GRAPHS OF PHOTON-INTERACTION CROSS SECTIONS FROM 0.1 keV TO 100 MeV DERIVED FROM THE LLL EVALUATED- NUCLEAR-DATA LIBRARY

ABSTRACT

Energy-dependent evaluated photon interaction cross sections and related parameters are presented for elements H through Cf ($Z = 1-98$). Data are given over the energy range from 0.1 keV to 100 MeV. The related parameters include form factors and average energy deposits per collision (with and without fluorescence). Fluorescence information is given for all atomic shells that can emit a photon with a kinetic energy of 0.1 keV or more. In addition, the following macroscopic properties are given: total mean free path and energy deposit per centimeter. This information is derived from the Livermore Evaluated-Nuclear-Data Library (ENDL) as of October 1978.

1978 EDITION

The photon energy range now extends from 0.1 keV to 100 MeV. In previous editions, the range was from 1.0 keV to 100 MeV. Except for the last decade of the photon energy range (0.1 to 1.0 keV), the cross sections are identical with those of the 1975 edition.

SOURCES OF EVALUATED CROSS-SECTION DATA

The data for coherent, incoherent, photoelectric, pair-production, and total cross sections are presented on an energy grid that accurately defines the cross section between tabulated points by using log-log interpolation. Fluorescence information is given for all atomic shells with photoelectric absorption edges of 0.1 keV or more.

FORM FACTORS, COHERENT CROSS SECTIONS, AND INCOHERENT CROSS SECTIONS

The form factors presented here are those of Hubbell et al.¹ Coherent and incoherent cross sections were obtained by integrating the angular distributions derived from the form factors. Log-log quadratic interpolation was used for the integration, as recommended in Ref. 1. The resulting cross sections differ somewhat from those one would obtain using simple log-log interpolation.

PAIR-PRODUCTION CROSS SECTIONS

The pair-production cross sections are basically those of Hubbell and Berger,² interpolated to the appropriate energy grid and extrapolated from $Z = 92$ to $Z = 98$.

PHOTOELECTRIC CROSS SECTIONS

The photoelectric cross sections for $Z = 84, 85, 87-89, 91, 93$, and $95-98$ are taken from the work of Storm and Israel.³ The evaluated data for the remaining 87 elements are those of McMasters et al.⁴ below 1 MeV and those of Hubbell and Berger² above 1 MeV (normalized to the McMasters et al.⁴ values at 1 MeV). The photoelectric cross sections below 1.0 keV were derived from the works of Scofield⁵ and Veigele⁶ for all elements.

FLUORESCENCE DATA^{3, 4, 7-13}

The photoelectric absorption edges for photon energies greater than 1 keV are derived from the jumps in the photoelectric cross sections of either Storm and Israel³ or McMasters et al.⁴ for each specific atomic number, as defined above. The energies of the photoelectric absorption edges between 0.1 and 1.0 keV are derived from either the jumps in the photoelectric cross sections or the tables of Storm and Israel³ if the cross sections did not permit unambiguous identification of the edges. Only edges at 0.1 keV or higher energy are presented.

Photoelectric cross sections for individual shells have not been widely measured over a significant range of energy or atomic number. We have used theoretical calculations⁷ to develop a systematic method of predicting the probability of a vacancy for each shell. Specifically, we used the ratio of the photoelectric cross section above each edge to that below it (i.e., the jump ratio) to define the vacancy probability for each shell. These probabilities are then assumed to be energy independent (e.g., above the K edge the photoelectric cross section is energy dependent, although the ratio of cross sections for individual shells are energy independent). Vacancy probabilities are only given for edges above 0.1 keV; therefore, if the sum of the vacancy probabilities from all shells is not one, it is because the remaining edges lie below 0.1 keV.

If we define the jump ratios for the K, L, and M edges as

$$\begin{aligned} P_K &= \frac{\sigma_{pe}(\epsilon_K + \delta)}{\sigma_{pe}(\epsilon_K - \delta)}, & (\text{product over 3 subshells}), \\ P_L &= \prod_{i=1,3} \frac{\sigma_{pe}(\epsilon_{L-i} + \delta)}{\sigma_{pe}(\epsilon_{L-i} - \delta)} & (\text{product over 3 subshells}), \\ P_M &= \prod_{i=1,5} \frac{\sigma_{pe}(\epsilon_{M-i} + \delta)}{\sigma_{pe}(\epsilon_{M-i} - \delta)} & (\text{product over 5 subshells}), \end{aligned} \quad (1)$$

then the vacancy probabilities for incident photon energies above the K edge are

$$\begin{aligned} V_K &= (1 - 1/P_K), \\ V_L &= (1 - 1/P_L)/P_K, \\ V_M &= (1 - 1/P_M)/(P_K P_L). \end{aligned} \quad (2)$$

Similarly, for incident photon energies below the K edge,

$$\begin{aligned} V'_L &= (1 - 1/P'_L), \\ V'_M &= (1 - 1/P'_M)/P'_L. \end{aligned} \quad (3)$$

For a vacancy in any given shell, the atom may emit either fluorescence or an Auger electron.⁹ Auger electrons are predominant for low-Z elements, and fluorescence is predominant for high-Z elements. Because of the subshell structure, the actual distribution of vacancies depends on the energy of the incident photon, which, in turn, affects the competition between fluorescence and Auger.⁸ Therefore, fluorescence probability for the L shell is given for two incident photon energy ranges ($E > K$, $K > E > L$).

The fluorescence transitions considered in this report are

$$(\infty) \rightarrow (M-v) \rightarrow (L-iii) \rightarrow (K) ,$$

$$(\infty) \rightarrow (M-iv) \rightarrow (L-ii) \rightarrow (K) , \quad (4)$$

$$(\infty) \rightarrow (M-iii) \rightarrow (K) .$$

The three transitions that are energetically most important in the filling of a K-shell vacancy are given for each atomic number. In the case of an L-shell vacancy, the probability of L-ii and L-iii vacancies may be assumed to be 0.371 and 0.629, respectively, independent of atomic number. In the case of an M-shell vacancy, a vacancy in all subshells may be considered equally probable. This prescription is adequate to describe most important transitions to within the uncertainty of the available fluorescence data.

PROCEDURES USED TO DERIVE DATA

The data that were derived from the ENDL photon-interaction cross section include total mean free path, energy deposit (with and without fluorescence), and the bremsstrahlung energy radiated by the electron.

TOTAL MEAN FREE PATH

The total mean free path is derived from the total microscopic cross section via the relationship

$$\lambda_R(\epsilon) = \frac{A}{\rho N_0 \sigma_t(\epsilon)} \text{ (cm)} , \quad (5)$$

where

A = atomic weight (based on $C^{12} = 12$),

ρ = density in g/cm^3 ,

N_0 = Avogadro's number ($0.6022169 \times 10^{24} \text{ mole}^{-1}$),

$\sigma_t(\epsilon)$ = microscopic total cross section in barns.

Both the atomic number and the density used in this calculation are given in the data tables. Standard temperature and pressure (STP) values of the density are used when available. If the density was unknown or poorly known, a value of 13.5 g/cm^3 is assumed and is indicated as ASSUMED DENSITY on plots.

ENERGY DEPOSITION

For an incident photon of energy ϵ (MeV), the average deposit for each reaction is calculated below.

Incoherent Energy Deposition

$$E_{inc}(\epsilon) = \frac{\int_{-1}^{+1} P(\epsilon, \mu) [\epsilon - \epsilon(\mu)] d\mu}{\int_{-1}^{+1} P(\epsilon, \mu) d\mu}, \quad (6)$$

where

μ = cosine of the scattering angle,

$P(\epsilon, \mu)$ = probability of the photon scattering through an angle whose cosine is μ ,

$$\epsilon(\mu) = \frac{\epsilon}{1 + \frac{\epsilon}{0.511}(1 - \mu)} = \text{exact energy-angle correlation.} \quad (7)$$

Coherent Energy Deposition

By definition of "coherent," no energy loss occurs.

Pair-Production Energy Deposition

$$E_{pp} = \epsilon - 1.022. \quad (8)$$

The remaining 1.022 MeV is the energy equivalent of the mass of the electron and the positron.

Photoelectric Energy Deposition

$$E_{pe} = \epsilon. \quad (9)$$

Unlike all the preceding processes, in which the energy deposit is electron or positron kinetic energy, the photoelectric process leads to electron kinetic energy and, possibly, to fluorescence. The sum of the kinetic energy deposit and the fluorescence energy deposit per collision is therefore

$$E_t(\epsilon) = \frac{E_{inc}(\epsilon) \sigma_{inc}(\epsilon) + \epsilon \sigma_{pe}(\epsilon) + (\epsilon - 1.022) \sigma_{pp}(\epsilon)}{\sigma_t(\epsilon)}. \quad (10)$$

By defining $F(\epsilon)$ as the fluorescence energy deposit per collision, the kinetic energy deposit per collision is less than the above energy deposit and is simply given by

$$E_{ke}(\epsilon) = E_t(\epsilon) - \frac{F(\epsilon) \sigma_{pe}(\epsilon)}{\sigma_t(\epsilon)}. \quad (11)$$

The value of $F(\epsilon)$ may be derived from the data in the volume by defining

E_i = Binding energy of the i th absorption edge (see pp. 491-497).

V_{ij} = Probability of creating a vacancy in the J shell (see pp. 498-501) when an incident photon has an energy in the range $E_i > E > E_{i-1}$.

F_{ij} = Probability of fluorescence when an incident photon has an energy in the range $E_i < E < E_{i-1}$, given a vacancy in the J shell (i.e., competition between fluorescence and Auger; see pp. 502-503).

T_{ij} = Transition probability from subshell i to shell K (see pp. 504-505) when an incident photon has an energy in the range $E_K < E$. All subsequent transition probabilities and transitions of photons with incident energies $E < E_K$ are independent of atomic number. $T_{L-iii, K-iv}$ is 0.629, $T_{L-ii, M-iv}$ is 0.371, and the transition probability from all M subshells are equally probable ($T_{M-i, \infty} = \dots = T_{M-v, \infty} = 1/5$).

The amount of photo. energy in fluorescence is

$$\begin{aligned}
& \underline{E > E_K} \\
F(e) = & V_{K,K} F_{K,K} T_{K,L-ii} \left\{ (E_K - E_{L-iii}) + F_{K,L} [(E_{L-iii} - E_{M-v}) + F_{K,M} (E_{M-v})] \right\} \\
& + V_{K,K} F_{K,K} T_{K,L-ii} \left\{ (E_K - E_{L-ii}) + F_{K,L} [(E_{L-ii} - E_{M-iv}) + F_{K,M} (E_{M-iv})] \right\} \\
& + V_{K,K} F_{K,K} T_{K,M-iii} \left\{ (E_K - E_{M-iv}) + F_{K,M} (E_{M-iii}) \right\} \\
& + V_{K,L} F_{K,L} (0.629) \left\{ (E_{L-iii} - E_{M-v}) + F_{K,N} (E_{M-v}) \right\} \\
& + V_{K,L} F_{K,L} (0.371) \left\{ (E_{L-ii} - E_{M-iv}) + F_{K,M} (E_{M-iv}) \right\} \\
& + V_{K,M} F_{K,M} \left(\frac{1}{5} \right) \left\{ E_{M-i} + E_{M-ii} + E_{M-iii} + E_{M-iv} + E_{M-v} \right\} . \quad (12)
\end{aligned}$$

$$\begin{aligned}
& \underline{F_K > E > E_{L-iii}} \\
F(e) = & V_{L,L} F_{L,L} (0.629) \left\{ (E_{L-iii} - E_{M-v}) + F_{L,M} (E_{M-v}) \right\} \\
& + V_{L,L} F_{L,L} (0.371) \left\{ (E_{L-ii} - E_{M-iv}) + F_{L,M} (E_{M-iv}) \right\} \\
& + V_{L,M} F_{L,M} \left(\frac{1}{5} \right) \left\{ E_{M-i} + E_{M-ii} + E_{M-iii} + E_{M-iv} + E_{M-v} \right\} . \quad (13)
\end{aligned}$$

$$\begin{aligned}
& \underline{E_{L-iii} > E > E_{M-v}} \\
F(e) = & F_{M,M} \left(\frac{1}{5} \right) \left\{ E_{M-i} + E_{M-ii} + E_{M-iii} + E_{M-iv} + E_{M-v} \right\} . \quad (14)
\end{aligned}$$

BREMSSTRAHLUNG ENERGY

Part of the electron kinetic energy (MeV/collision) will be deposited by ionization (or leak from the system), and part will be re-emitted as bremsstrahlung energy. For electrons, the ratio of bremsstrahlung to ionization energy loss per unit track length is approximately⁹

$$\frac{(dT/dS)_{\text{rad}}}{(dT/dS)_{\text{ion}}} \approx \frac{ZT}{800} \quad (15)$$

integrated over the entire track length of the electron, the total energy loss due to ionization and bremsstrahlung will be approximately

$$E_{\text{ion}} = \frac{E}{1 + \frac{ZE}{1600}} \quad (16)$$

$$E_{\text{rad}} = \frac{\frac{ZE^2}{1600}}{1 + \frac{ZE}{1600}} \quad (17)$$

Equation (17) has been used to estimate the bremsstrahlung.

TABLE AND GRAPH CONVENTIONS

The pair production at 1.022 MeV has been arbitrarily set to 10^{-6} barns. Individual cross sections less than 10^{-5} barns, or less than $\pm \times 10^{-4}$ of the total cross section, are not included on the plots.

PRODUCTION OF THE VOLUME

The graphs and tables in this volume were produced by the program PHOTONPLOT.¹⁴ The program required a single noninteractive pass through the ENDL photon-interaction cross-section library, requiring 1.6 min of CDC 7600 time, to produce a single roll of 35-mm film and 105-mm microfiche containing all graphs and tables in correct atomic number order, ready for photo-offset printing.

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