ornl

OAK
RIDGE
NATIONAL
LABORATORY

UNION
CARBIDE

ORNL/RSIC-46
(ENDF-335)

Description of the DLC-99/HUGO Package of Photon Interaction Data in ENDF/B-V Format

R. W. Roussin
J. R. Knight
J. H. Hubbell
R. J. Howerton

RADIATION SHIELDING INFORMATION CENTER

OPERATED BY
UNION CARBIDE CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A03; Microfiche A01

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ORNL/RSIC-46
(ENDF-335)

Contract No. W-7405-eng-26

Engineering Physics Division
Radiation Shielding Information Center

DESCRIPTION OF THE DLC-99/HUGO PACKAGE OF PHOTON INTERACTION DATA IN ENDF/B-V FORMAT

R. W. Roussin
Radiation Shielding Information Center

J. R. Knight
Computer Sciences Division

J. H. Hubbell
National Bureau of Standards
Washington, DC

R. J. Howerton
Lawrence Livermore National Laboratory
Livermore, California

Research sponsored by

Department of Energy-Office of Reactor Research and Technology
Department of Energy-Office of Military Applications
and
Defense Nuclear Agency
Interagency agreement no. 42 87 10 30 1

Date Published: December 1983

NOTICE This document contains information of a preliminary nature. It is subject to revision or correction and therefore does not represent a final report.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
operated by
UNION CARBIDE CORPORATION
for the
U.S. DEPARTMENT OF ENERGY

Table of Contents

	Page
Abstract	1
Introduction	1
Features of the New Evaluation	2
Comparison of DLC-99/HUGO and DLC-7/HPICE	4
Contents of the DLC-99/HUGO Package	13
References	14
Appendix A: History of the DLC-7/HPICE Library	16
Appendix B: The EDPHOT and COMP23 Computer Codes for Editing and Comparing Photon Interaction Data in ENDF Format.	17

Description of the DLC-99/HUGO Package of Photon Interaction Data in ENDF/B-V Format

R. W. Roussin, J. R. Knight*, J. H. Hubbell,**
and R. J. Howerton***

ABSTRACT

A new photon interaction data library, DLC-99/HUGO, is described. The library was prepared by incorporating newly evaluated data from the National Bureau of Standards with that from an existing data library, DLC-7F/HPICE, which is the ENDF/B-IV photon interaction data. It contains pair and triplet cross sections, photoelectric cross sections, and atomic form factors and the corresponding coherent scattering cross sections. Evaluated data in ENDF/B-V format are provided for elements Z=1 to 100. The data package, available from the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory, will be submitted to CSEWG for consideration as the ENDF/B-V Photon Interaction Library. Two computer codes, EDPHOT for selectively printing the data and COMP23 for comparing two photon interaction libraries, are also provided.

INTRODUCTION

A photon interaction data library was first placed in the Radiation Shielding Information Center (RSIC) Data Library Collection (DLC)[1] in 1969. The evaluation was based on work by McMaster et al.[2] and Plechaty and Terrall[3] and made available in ENDF format.[4] Designated DLC-7/HPICE, the data compilation served, with minor modification, as the CSEWG-approved photon interaction library for the Evaluated Nuclear Data File for ENDF/B-II and -III.[5] In 1975 an extensive revision was made based on the work of Hubbell et al.[6] and the resulting data library, DLC-7E, with minor modifications, served as the ENDF/B-IV[7] photon interaction data. The history of the DLC-7 series is summarized in Appendix A.

---

*Computer Sciences Division, Oak Ridge National Laboratory.
**National Bureau of Standards.
***Lawrence Livermore National Laboratory.

The new data library, DLC-99/HUGO, a major revision of the basic data library excerpted from data compiled at NBS by one of the authors (J. H. Hubbell), has been placed in the ENDF/B-V format[8] and is intended to serve as the ENDF/B-V[9] photon interaction data. As with the DLC-7 series, the current library was assembled by a collaboration of the principal evaluators and RSIC. During this exercise, an editing computer code (EDPHOT) was modified and updated to handle ENDF/B-V formats and was used to compare and examine the data. In addition, another computer code (COMP23) was used in detailed comparisons to compare DLC-99 with DLC-7. Both are included as part of the package.

FEATURES OF THE NEW EVALUATION

General

Data are provided for elements Z=1 to 100. Both cross-section data (ENDF file 23) and coherent scattering form factors and incoherent scattering functions (ENDF file 27) are included as part of the same library. The cross section energy range is 1 keV to 100 MeV. The scattering function and form factor data are tabulated as a function of inverse angstroms over the range from 0 to 10^9 Å^{-1}.

The DLC-99/HUGO data are in ENDF/B-V format. There is no practical difference between the data representation for photon interactions in ENDF/B-IV and -V. The user may need to modify existing programs that now access DLC-7 in order to properly read an extra record at the start of each material in DLC-99. There is additional information allowed in the dictionary in the ENDF/B-V format. The parameter, MOD, can be used to indicate that the data set for a particular reaction is carried over from the previous version (MOD=0), is new for this version (MOD=1), or has been revised (MOD>1) since the release of the particular version of ENDF/B.

Discussion of Individual Processes

A brief description of the sources of evaluated data for the various photon interaction processes included in DLC-99 are given in the sections that follow.

Coherent Scattering

The relativistic atomic form factors and corresponding photon coherent scattering cross sections of Hubbell and Øverbø[10] were used for the MF=27,MT=502, and MF=23,MT=502 data, respectively, in DLC-99/HUGO. These provide new values for the ENDF/B-V library.

Incoherent Scattering

Incoherent scattering functions and corresponding incoherent scattering cross sections of Hubbell et al.[6] were used for the MF=27,MT=504 and MF=23,MT=504 data, respectively. These are the same as were used for DLC-7E, the ENDF/B-IV file. Data for helium, however, have been revised slightly for DLC-99/HUGO in order to incorporate a revision published by Hubbell[11] in 1977.

Pair and Triplet Production

For DLC-99, the components of electron-positron pair production cross sections are provided as MF=23,MT=515 (pair production electron field) and MF=23,MT=517 (pair production nuclear field). A total production cross section is also provided (MF=23,MT=516) as the sum of the two components. The data were taken from the work of Hubbell, Gimm, and Øverbø.[12] The data for MT=517 refer to coherent production where the atom recoils without internal excitation, and MT=515 refers to incoherent production in which the atom is either excited or ionized (triplet production). These components were not explicitly provided in DLC-7.

Photoelectric Cross Section

The photoelectric cross sections were evaluated based on the theoretical work of Scofield[13] using procedures described and implemented by Hubbell et al.[6,14,15] The data are presented as MF=23, MT=602.

COMPARISON OF DLC-99/HUGO AND DLC-7/HPICE

While the overall knowledge of photon interaction cross sections is much better than that for neutrons, the recent evaluation work cited in the references to this report reflect refinements which are worth incorporating into calculational schemes used for radiation transport analysis. To give a general feel for the qualitative changes between DLC-99 and DLC-7, some comparison plots are provided.

The photoelectric (MT=602), coherent scattering (MT=502) and total pair production (MT=516) cross sections from DLC-99 and DLC-7 are shown for hydrogen, beryllium, iron, lead, and uranium in Figs. 1-5, respectively. More detail in the photoelectric cross section for iron, lead, and uranium are shown in Figs. 6-8, respectively.

During the preparation of DLC-99, detailed comparisons between the two data libraries were made. In general, the maximum change in the coherent scattering cross section for DLC-99 ranged from about 1% higher for iron to 16% higher for plutonium, with the low-Z materials being essentially the same. The total pair production cross section for DLC-99 is also higher, ranging from a maximum of about 3% for low-Z to about 12% for high-Z, the maximum difference occurring in the 1 to 3 MeV region. The photoelectric process shows large systematic differences for the low-Z materials for energies above 1 MeV, DLC-99 being higher. In addition, for high-Z materials at low energy, in the vicinity of absorption edges, some substantial differences are seen. These are usually due to refinements in the precise location of the edges between the two libraries.

ORNL-DWG 83-18146

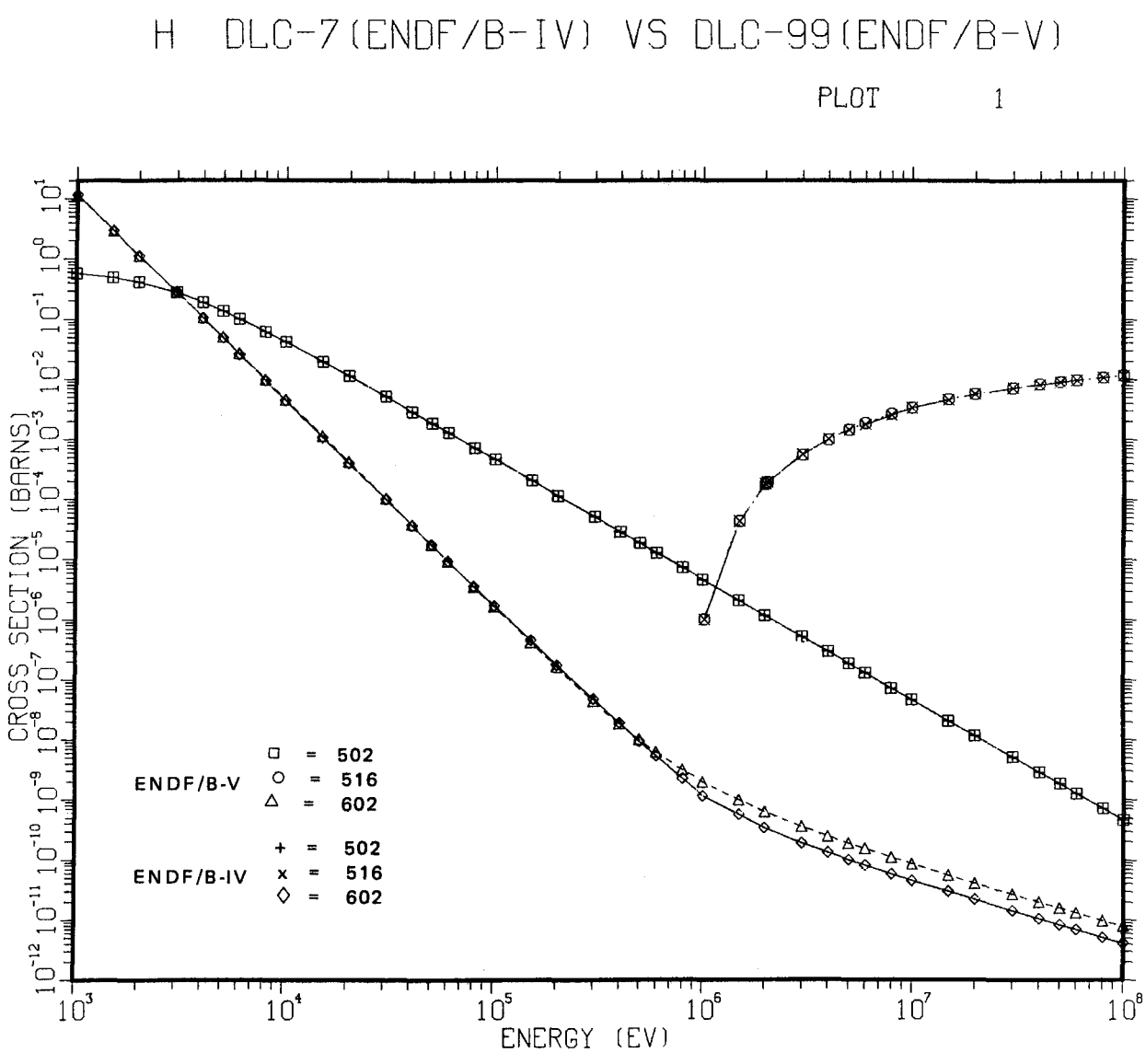

Fig. 1. Comparison of DLC-7/HPICE and DLC-99/HUGO coherent (MT=502), production (MT=516) and photoelectric (MT=602) cross sections for hydrogen.

ORNL-DWG 83-18147

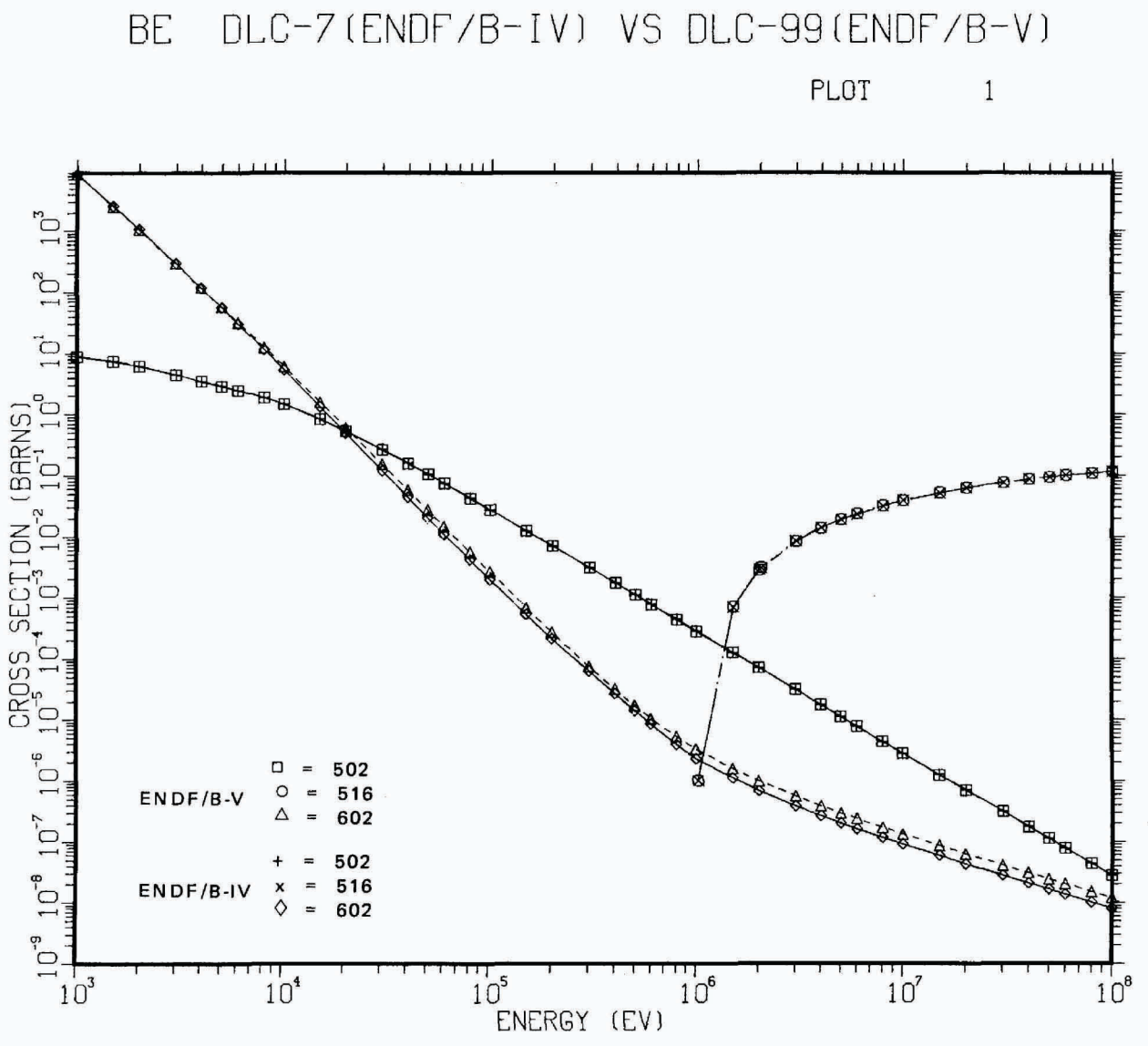

Fig. 2. Comparison of DLC-7/HPICE and DLC-99/HUGO coherent (MT=502), production (MT=516) and photoelectric (MT=602) cross sections for beryllium.

ORNL-DWG 83-18148

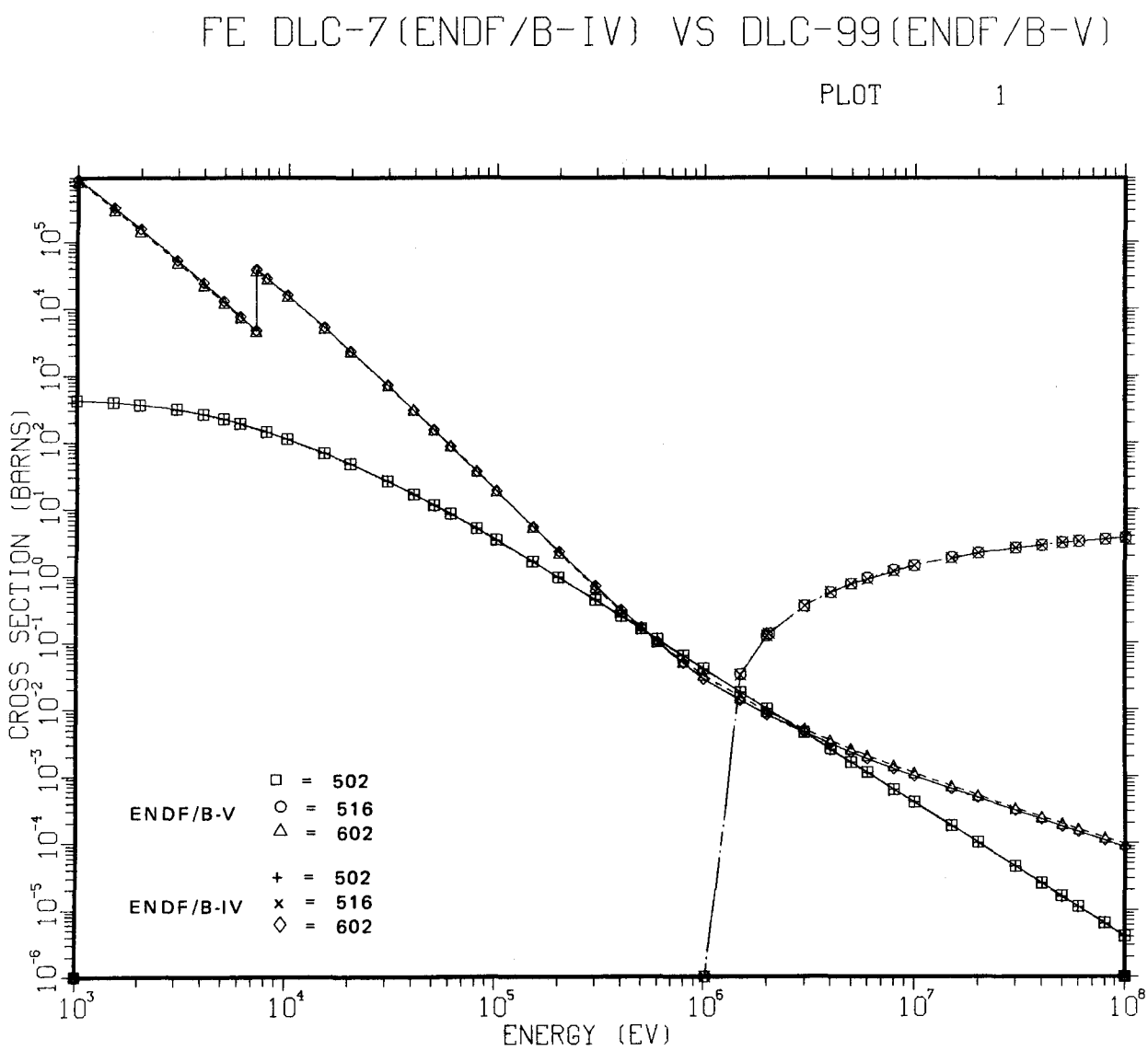

Fig. 3. Comparison of DLC-7/HPICE and DLC-99/HUGO coherent (MT=502), production (MT=516) and photoelectric (MT=602) cross sections for iron.

ORNL-DWG 83-18149

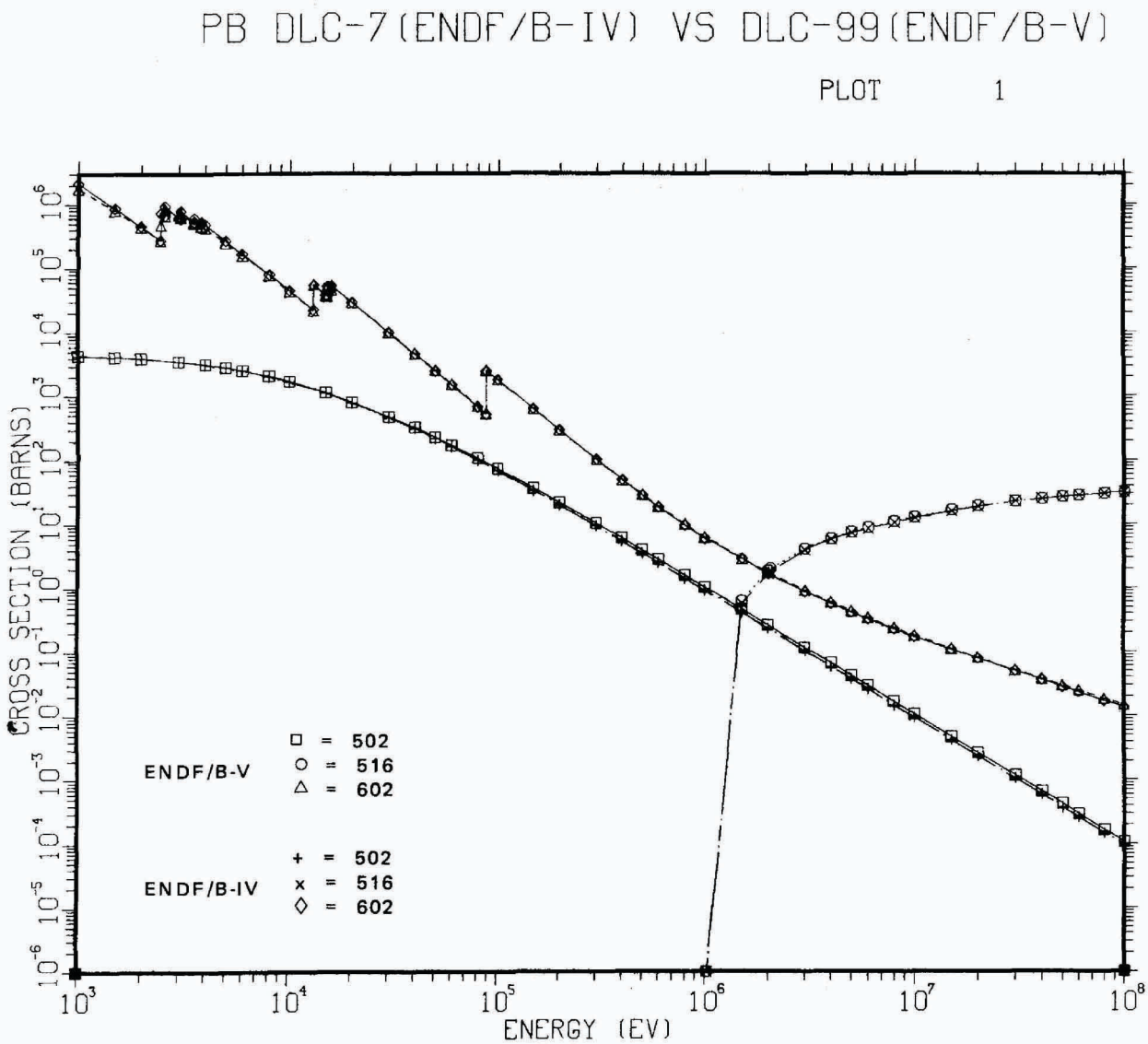

Fig. 4. Comparison of DLC-7/HPICE and DLC-99/HUGO coherent (MT=502), production (MT=516) and photoelectric (MT=602) cross sections for lead.

ORNL-DWG 83-18150

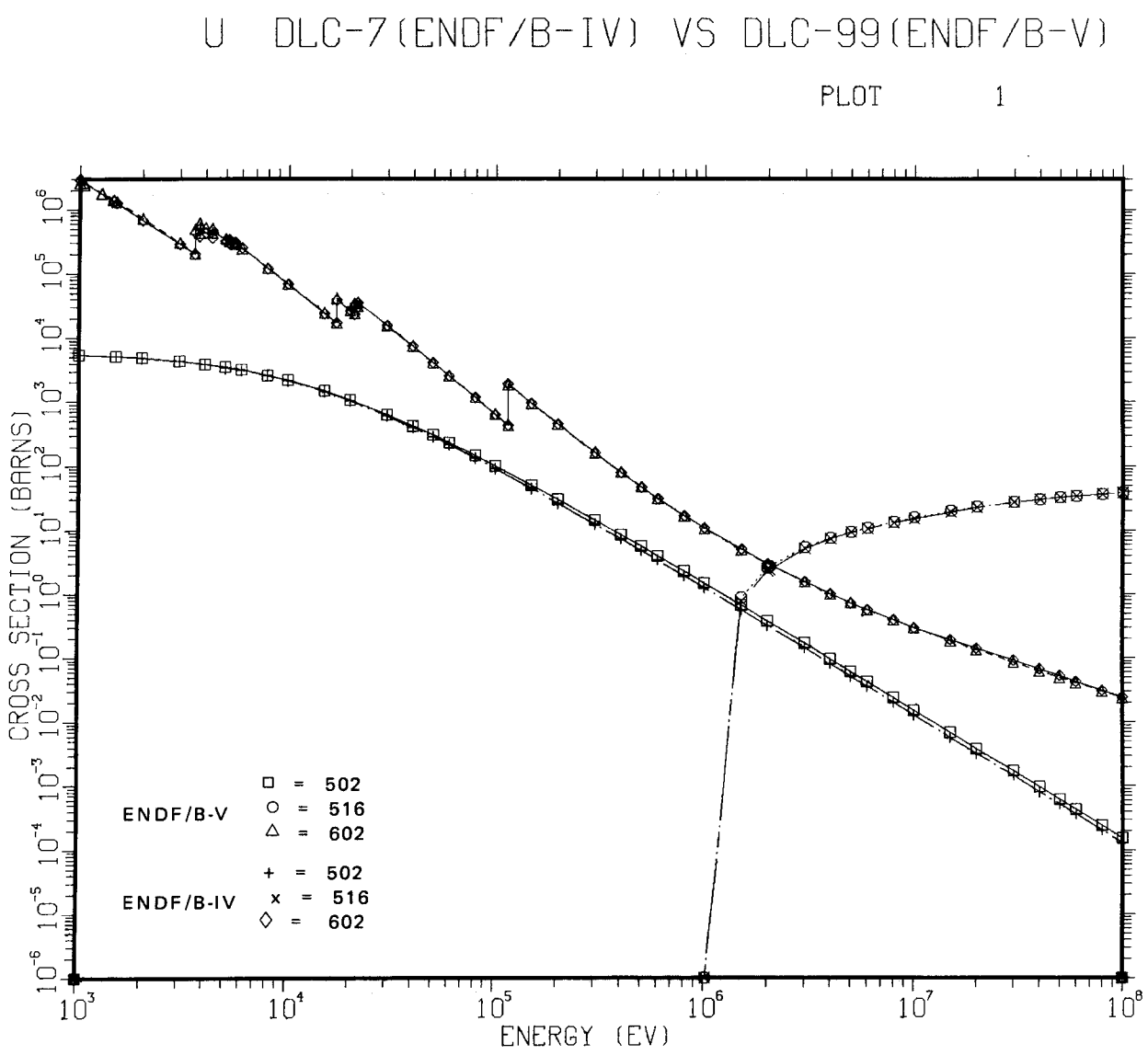

Fig. 5. Comparison of DLC-7/HPICE and DLC-99/HUGO coherent (MT=502), production (MT=516) and photoelectric (MT=602) cross sections for uranium.

ORNL-DWG 83-18151

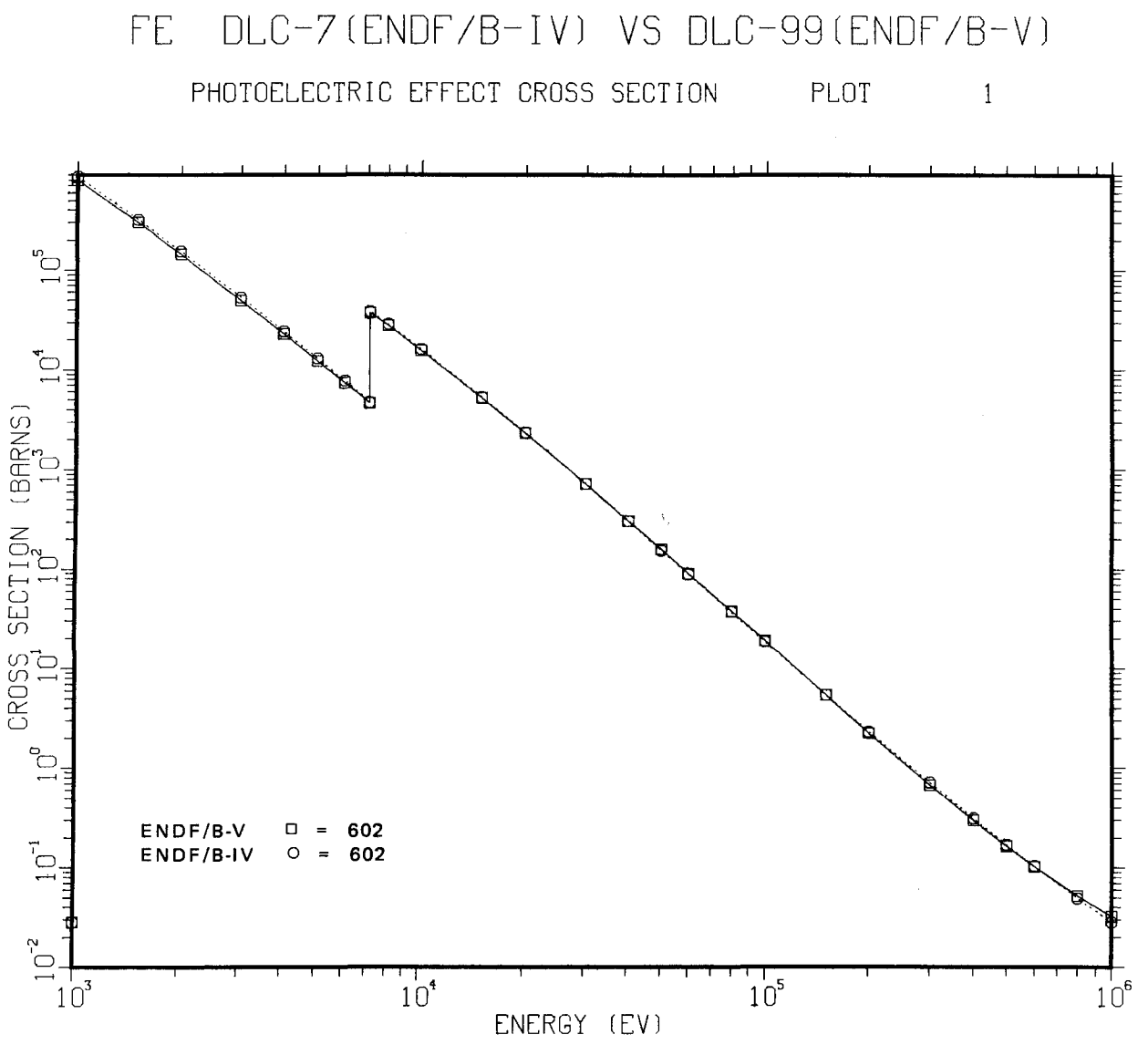

Fig. 6. Detailed comparison of DLC-7/HPICE and DLC-99/HUGO photoelectric cross sections for iron.

ORNL-DWG 83-18152

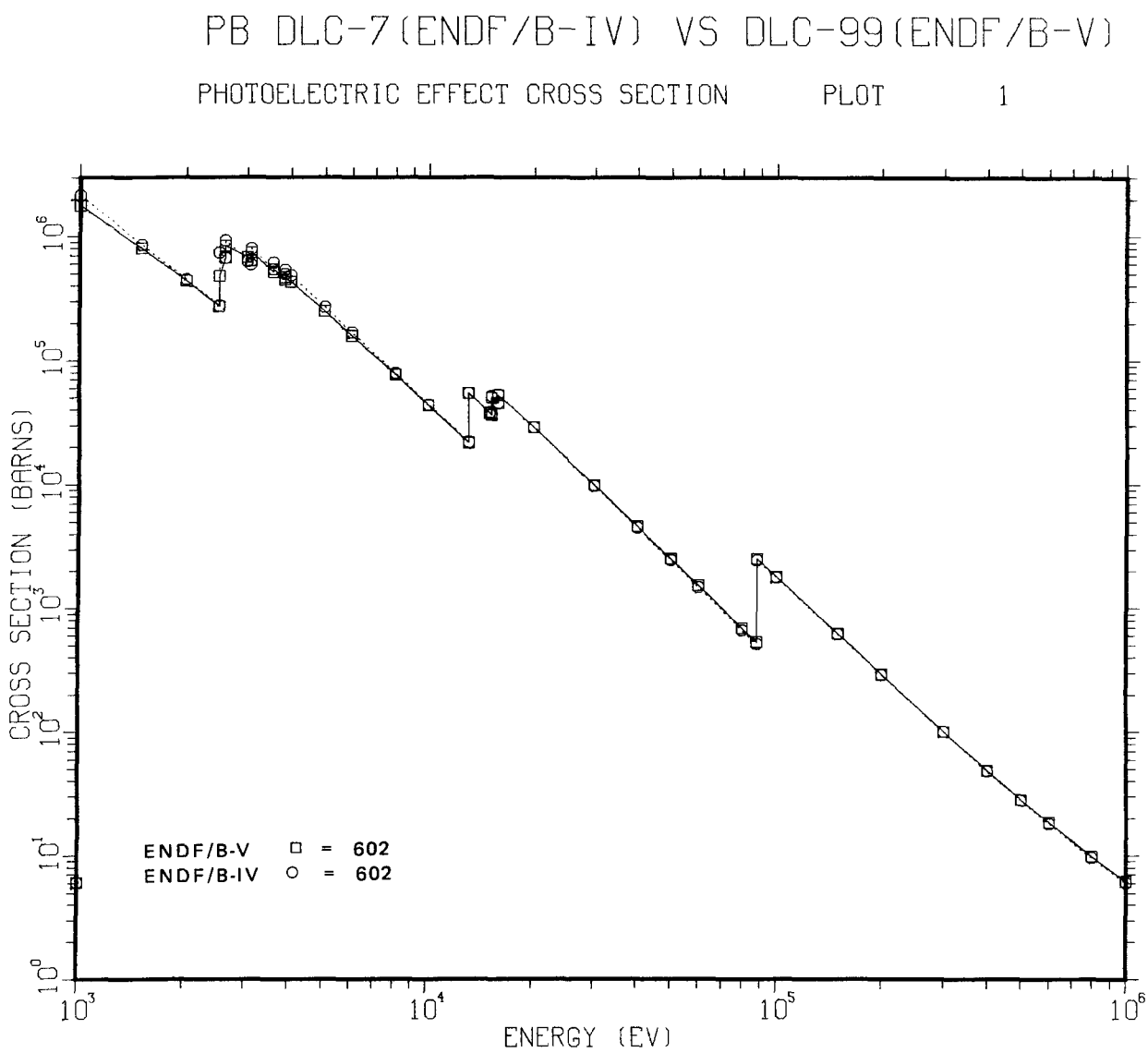

Fig. 7. Detailed comparison of DLC-7/HPICE and DLC-99/HUGO photoelectric cross sections for lead.

ORNL-DWG 83-18153

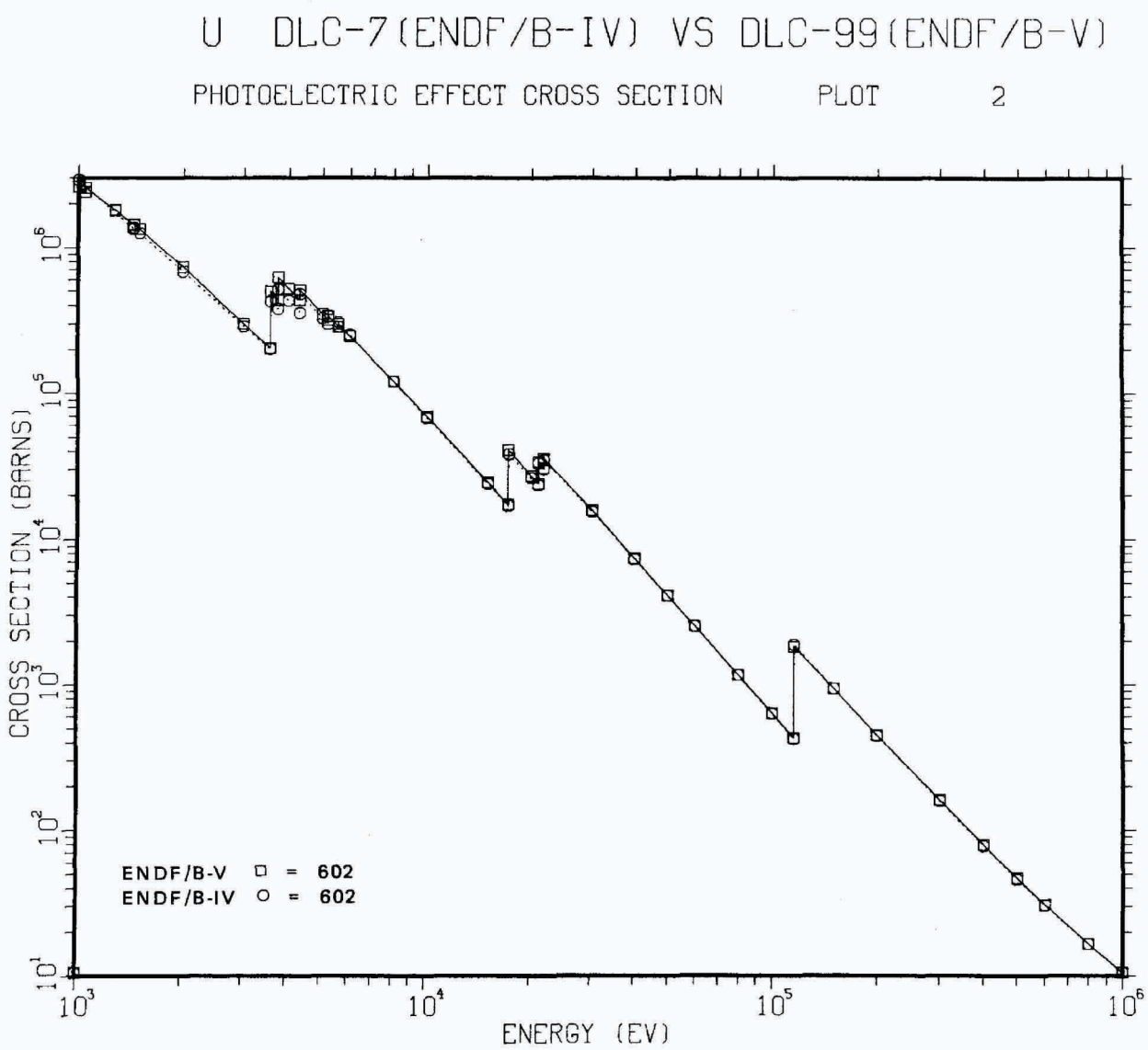

Fig. 8. Detailed comparison of DLC-7/HPICE and DLC-99/HUGO photoelectric cross sections for uranium.

CONTENTS OF THE DLC-99/HUGO PACKAGE

The DLC-99/HUGO package can be obtained by mailing a 2400-ft reel of magnetic tape to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, TN 37830

The package contains the photon interaction library in ENDF/B-V format for materials Z=1 through 100. Two programs are provided for editing and comparing the data, EDPHOT and COMP23, respectively. A brief description of the codes is provided in Appendix B. Sample input and output are also provided in the package to demonstrate the use of the codes.

The general contents of the data library are given in Table 1.

Table 1. Structure and contents of the data files given for each element in DLC-99

Number		Description
File	Reaction	
MF	MT	
1	451	Hollerith description of the data
23	501	Total cross section
23	502	Coherent scattering cross section
23	504	Incoherent scattering cross section
23	515	Incoherent pair production cross section (triplet)
23	516	Total pair production cross section
23	517	Coherent pair production cross section
23	602	Photoelectric cross section
27	502	Coherent scattering form factors
27	504	Incoherent scattering functions

REFERENCES

1. R. W. Roussin, Abstracts of the Data Library Packages Assembled by the Radiation Shielding Information Center, ORNL/RSIC-30/V1 (1972).
2. W. H. McMaster, N. K. Del Grande, J. H. Mallett, and J. H. Hubbell, Compilation of X-Ray Cross Sections, UCRL-50174, Sect. I (Jan. 1970), Sect. II, Rev. 1 (May 1969), Sect. III (Aug. 1969).
3. E. F. Plechaty and J. R. Terrall, Photon Cross Sections 1 keV to 100 MeV, UCRL-50400, Vol. VI (1968).
4. D. Garber, C. Dunford, and S. Pearlstein, ENDF 102 Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF, BNL-NCS-50496 (ENDF-102) (1975).
5. O. Ozer and D. Garber, ENDF 201 ENDF/B Summary Documentation, BNL-17541 (ENDF 201) (ENDF/B-III) (1973).
6. J. H. Hubbell, W. J. Veigele, E. Briggs, R. T. Brown, D. T. Cromer, and R. J. Howerton, "Atomic Form Factors, Incoherent Scattering Functions and Photon Scattering Cross Sections," J. Phys. Chem. Ref. Data, 4: 471 (1975).
7. D. Garber, ENDF-201 ENDF/B Summary Documentation, BNL 17541 (ENDF-201) (ENDF/B-IV) (1975).
8. R. Kinsey, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF, BNL-NCS-50496 (ENDF-102) 2d. ed. (ENDF/B-V)(1969).
9. R. Kinsey, ENDF-201 ENDF/B Summary Documentation, BNL-NCS-17541 (ENDF-201) 3d. ed. (ENDF/B-V)(1979).
10. J. H. Hubbell and I. Øverbø, "Relativistic Atomic Form Factors and Photon Coherent Scattering Cross Sections," J. Phys. Chem. Ref. Data, 8: 89 (1979).
11. J. H. Hubbell, "Erratum to Atomic Form Factors, Incoherent Scattering Functions and Photon Scattering Cross Sections," J. Phys. Chem. Ref. Data, 6:615 (1977).
12. J. H. Hubbell, H. A. Gimm, and I. Øverbø, "Pair, Triplet and Total Atomic Cross Sections for 1 MeV--100GeV Photons in Elements Z=1 to 100," J. Phys. Chem. Ref. Data, 9: 1023 (1980).

13. J. H. Scofield, Theoretical Photoionization Cross Sections from 1 to 1500 keV, UCRL-51326 (1973).

14. J. H. Hubbell, "Photon Mass Attenuation and Mass Energy Absorption Coefficients for H, C, N, O, Ar, and Seven Mixtures from 0.1 keV to 20 MeV," Rad. Research, 70: 58 (1977).

15. J. H. Hubbell, "Photon Mass Attenuation and Mass Energy Absorption Coefficients from 1 keV to 20 MeV," Intl. J. Appl. Rad. Isotopes, (Oct. 1982).

APPENDIX A. History of the DLC-7/HPICE Library

The DLC-7/HPICE data package has been modified several times since its initial release. Various versions of the data library have served as the official ENDF/B Photon Interaction Data Library. A summary of this historical information is provided in Table A1.

Table A1. History of the DLC-7/HPICE data package

Designation	Date	ENDF/B version	Comments
DLC-7	Sept. 1969		Initial release.
DLC-7C	Jan. 1970	ENDF/B-II	Named ENDF/B-II photon interaction data library.
DLC-7D	Apr. 1971	ENDF/B-III	Pair production increased by 3-5% at 4 MeV for all Z; incoherent scattering corrected at 0.8 MeV for Z=31 to 34.
DLC-7E	July 1975	ENDF/B-IV	File 27 data added & corresponding file 23 cross sections replaced existing ones.
DLC-7F	Oct. 1975	ENDF/B-IV	File 23 data for coherent and incoherent scattering changed slightly due to use of 1973 Fundamental Constants.*

*E. R. Cohen and B. N. Taylor, "The 1973 Least-Squares Adjustment of the Fundamental Constants," J. Phys. Chem. Ref. Data, (2) 4: 663 (1973).

APPENDIX B. The EDPHOT and COMP23 Computer Codes for Editing* and Comparing Photon Interaction Data in ENDF Format

EDPHOT: A Computer Code for Editing Photon Interaction Data in ENDF Format

The EDPHOT computer code was developed by modifying an ENDF plotting and editing computer code, PLOTFB,[1] to edit photon interaction data. Since PLOTFB is very general, the EDPHOT program is somewhat inefficient and the coding difficult to follow. It can, however, provide edits of both MF=23 cross sections and MF=27 coherent scattering form factors and incoherent scattering functions. An earlier version of EDPHOT, EDIT-23, is available in the DLC-7/HPICE data package.

EDPHOT Input Data

A) Option Card

The input cards to the program consist of one card specifying the input, output options for the program, followed by up to 50 data requests. The contents of the first card and interpretation or restrictions are as follows (Format 6I5):

Field	
1	Logical number of ENDF/B input data unit (greater than zero).
2	Any number greater than zero.
3	Mode of the input tape (1 - BCD; 2 - BINARY).

*The word "edit" here means a selective printout of the data with meaningful labels.

4 ENDF/B tape label number (greater than zero - read and check tape label) (equal zero - read tape label; do not check it) (less than zero - do not read or check tape label).

5 Listing selector (1 - list output; not 1 - no listed output).

6 Editing selector (1 - each section starts at the top of a page) (not 1 - minimize the number of pages of output).

B) Data Request Cards

The data requests may identify a set of data by MAT and/or ZA number. Data may then be selected by file. Each data request card contains (Format I5,F10.0,5X,2I3):

Field

1 ENDF/B Material number (MAT).

2 ENDF/B ZA number (floating point: 1000.*Z + A)

3 The number 23 (for File 23 in the ENDF Format) is always punched in this field.

4 The number 27 (for File 27 in the ENDF Format).

The list of request cards must be terminated by a card having blank MAT and ZA fields.

To obtain the contents of an entire tape, the MAT and ZA fields of the first request card should be blank.

COMP23. A Computer Code for Editing and Comparing Two Photon Interaction Cross Section Libraries in ENDF Format

COMP23 can be used to edit and compare photon interaction cross sections from two libraries. It is useful in assessing the impact of changes when a new evaluation of photon interaction data is contemplated. The present version will compare only the cross-section

data (i.e., MF=23) in ENDF terminology. Most of the subroutines are standard ENDF retrieval routines.[1]

The "old" data are compared to the "new" data, a difference is calculated at each energy point and, if any deviation greater than the tolerance EPS is detected, the old, new, and difference are printed in tabular form. If necessary, the data sets are placed on a common energy grid by interpolation. The default tolerance is 1%.

The two libraries must be in the same ENDF mode, which can be either BCD or binary. The data may be in different format, i.e., ENDF/B-IV or -V.

COMP23 Logical Unit Assignment

"old" data	Logical Unit 1
"new" data	Logical Unit 2

COMP23 Input Data Requirements (2 cards)

Card 1. Format (I5,E10.3)

Field	
1	Mode of the two libraries (1 - library, 2 - BCD).
2	Tolerance of the comparison (0.01 - 1%). A zero or blank give default tolerance of 1%.

Card 2. Format (2I5)

Field	
1	Format of the "old" library (4 - ENDF/B-IV, 5 - ENDF/B-V).
2	Format for "new" library (4 - ENDF/B-IV, 5 - ENDF/B-V).

REFERENCE

1. O. Ozer, ed., ENDF-110, Description of the ENDF/B Processing Codes and Retrieval Subroutines, BNL 50300 (ENDF110) (1971), (Program PLOTFB by D. E. Cullen).

ORNL/RSIC-46
(ENDF-335)

INTERNAL DISTRIBUTION

1-2. Central Research Library
3. ORNL-Y-12 Technical Library Document Reference Section
4-5. Laboratory Records Department
6. Laboratory Records, ORNL R.C.
7. ORNL Patent Office
8-9. L. S. Abbott
10. R. G. Alsmiller
11. D. E. Bartine
12. G. F. Flanagan
13. W. E. Ford, III
14. N. M. Greene
15. J. L. Lucius
16. J. R. Knight
17. F. C. Maienschein
18. A. T. Malinauskas
19. R. W. Peelle
20. L. M. Petrie
21. M. W. Rosenthal
22. R. W. Roussin
23. D. B. Trauger
24. C. R. Weisbin
25. J. E. White
26. A. Zucker
27. P. W. Dickson, Jr. (Consultant)
28. J. C. Kouts (Consultant)
29. W. B. Lowenstein (Consultant)
30. R. Wilson (Consultant)
31-79. RSIC Distribution

EXTERNAL DISTRIBUTION

80. David L. Auton, Defense Nuclear Agency, Washington, DC 20305.
81. S. Berk, Office of Fusion Energy, U.S. DOE, Washington, DC 20545.
82. P. B. Hemmig, Office of Reactor Research and Technology, U.S. DOE, Washington, DC 20545.
83. R. J. Howerton, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550.
84. J. H. Hubbell, National Bureau of Standards, Center for Radiation Research, Washington, DC 20234.
85. J. W. Lewellen, Office of Reactor Research and Technology, U.S. DOE, Washington, DC 20545.
86. O. Ozer, Electric Power Research Institute, 3412 Hillview Ave., Palo Alto, CA 94304.
87. J. Renken, Sandia National Laboratories, P.O. Box 9336, Albuquerque, NM 87185.
88. Yo Taik Song, Office of Military Applications, U.S. DOE, Washington, DC 20545.
89. Myrna Steele, U.S. Nuclear Regulatory Commission, Washington, DC 20545.
90. W. L. Thompson, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87545.
91-184. National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973.
185-186. Technical Information Center, U.S. DOE, Oak Ridge, TN 37831.
187. Office of the Assistant Manager, Energy Research Development, DOE-ORO, Oak Ridge, TN 37831.
188. Patent Office, U.S. DOE, Oak Ridge, TN 37831.