LA-UR -78-771

CONF-780334--4

MASTER

TITLE: NJOY: A COMPREHENSIVE ENDF/B PROCESSING SYSTEM

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SUBMITTED TO: RSIC Multigroup Cross Section Seminar
Oak Ridge, Tennessee
March 14-16, 1978

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

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Form No. 836
St. No. 2629
1/78

UNITED STATES
ENERGY RESEARCH AND
DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

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NJOY: A COMPREHENSIVE ENDF/B PROCESSING SYSTEM

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ABSTRACT

NJOY is the successor to the MINX code. It provides an efficient and accurate capability for processing ENDF/B-IV and V data for use in fast reactor, thermal reactor, fusion reactor, shielding, and weapons analysis. NJOY produces neutron cross sections and group-to-group scattering matrices, heat production cross sections, photon production matrices, photon interaction cross sections and group-to-group matrices, delayed neutron spectra, thermal scattering cross sections and matrices, and cross-section covariances. Detailed pointwise cross sections, heating KERMA factors, thermal cross sections, and energy-to-energy thermal matrices are also available for plotting and Monte Carlo applications. NJOY currently processess all types of data on ENDF/B except for the decay chain and fission product yield files. NJOY provides output in the CCCC ISOTXS, BRKOXS, and DLAYXS formats, in DTF/ANISN format, and in a new comprehensive format called MATXS. Other important features of NJOY include free-format input, efficient binary I/O, dynamic storage allocation, an extremely modular structure, an accurate center-of-mass Gaussian integration for two-body scattering, and a flux calculator that makes it possible to compute accurate self-shielded cross sections when wide and intermediate-width resonance effects are important. NJOY is a single, integrated, efficient system that produces almost all of the basic cross sections required for multigroup methods of nuclear analysis.

INTRODUCTION

As data requirements for nuclear analysis grow steadily more complex, the analyst is faced with a bewildering variety of acronymic codes and libraries, each fulfilling only part of his needs, and each using a different format. Assembling the data he needs is full of annoyances, and incompatibilities are a constant danger. The goal of the NJOY development program has been to create a single self-consistent easy-to-use system which will process all data types in the ENDF/B evaluated nuclear data files[1] and output it in the form the designer needs.

NJOY is a child of MINX[2] and the name stands for "MINX-plus." It is a modular system where each module is an essentially free-standing code devoted to one particular processing task (see Table 1 for a list of the current modules. The following sections discuss the structure of NJOY and describe the functions and interesting features of each module.

Table 1. The Modules of NJOY

Name	Function
MODER	BCD/binary mode conversion
RECONR	Cross section reconstruction
BROADR	Doppler broadening
UNRESR	Unresolved cross sections
HEATR	Heating pointwise cross sections
THERMR	Thermal pointwise cross sections
GROUPR	Group neutron and nγ cross sections
GAMINR	Gamma interaction cross sections
ERRORR	Cross section covariances
DTFR	DTF format output
CCCCR	CCCC (Verion III) format output
MATXSR	MATXS format output

STRUCTURE AND UTILITIES

The overall structure of the NJOY system is shown in Fig. 1. All working modules communicate with each other using disk files (loosely "tapes") in ENDF/B format. These files are the original ENDF/B tape, a completely pointwise ENDF tape (PENDF), and a groupwise ENDF tape (GENDF). Modules can be run in many different orders and these internal tapes are useful for restarts. For example, a single saved GENDF tape can be reformatted into DTF, CCCC, and MATXS formats without rerunning the expensive group-averaging process. Similarly, multigroup constants for several different group structure and weighting function combinations can be run from one preprocessed PENDF tape.

The function of the main program is to specify the order of execution of these modules. In OVERLAY versions of the code, it also contains the library of utility systems available to all modules: free format input, variable-dimensioned dynamic storage, and ENDF/B input/output and computation.

NJOY contains its own machine-independent free format input processor with very simple rules of context. This input routine is especially useful with terminal-oriented computer systems. Variable-dimensioned storage and dynamic storage allocation are handled by a set of simple subroutines called the STORAG package. It allows space to be reserved, released, or located by name in a large container array. As a result, computer memory is used very efficiently.

The ENDF/B I/O routines in NJOY use either the BCD mode or a new blocked binary mode. The new mode allows large tabulations to be broken up into small logical records which can be "paged" through calculations efficiently without using excessive memory. Significant time savings are achieved by avoiding repeated "coding" and "cracking" of BCD records as shown in Table 2. MODER is used to convert back and forth between ENDF/B BCD and blocked binary modes.

Table 2. Comparison of BCD and Binary I/O Modes

Test	BCD	Binary
^{235}U Doppler broadening	169.0	72.1
^{235}U P_3 elastic matrix	10.9	4.99
^{235}U(n,2n) matrix	4.31	0.34
Fe Doppler broadening	139.	46.5

RECONR

This module reconstructs ENDF/B cross sections on a union energy grid such that all partial cross sections can be represented to within a stated accuracy using linear interpolation. The total cross section and any other summation cross sections (i.e., inelastic, sometimes fission, sometimes n,2n) are then recomputed to equal the sum of their parts. Linearization uses the method developed for MINX and resonance reconstruction uses the methods of RESEND[3] with several additions. A more efficient multilevel Breit-Wigner resonance calculation has been added based on the work of C. Lubitz.[4] The accurate Hwang and Henryson unresolved quadrature set[5] has been added. Finally, an option has been added to the single-level Breit-Wigner calculation to allow reconstruction at a specified temperature using the ψ and χ functions. The input to RECONR is a standard ENDF tape; the output is a PENDF tape.

BROADR

This module broadens tabulated cross sections at some input temperature to specified output temperatures. The results can be thinned to a specified accuracy. In the "bootstrap" mode, the starting temperature for final temperature 2 is final temperature 1. Due to the thinning, this mode is faster. Restart from a previously broadened PENDF tape is possible to add temperatures or to recover from an error in a previous attempt such as time limit.

The method of the SIGMA-1 code[6] is used with two major modifications. First, storage and indexing of data is changed to allow for broadening of several reactions on the union grid simultaneously. The summation cross

sections are recomputed after broadening. Second, a new method for computing broadening integrals at low energies and high temperatures is used which eliminates a numerical instability in the original code. Table 3 compares processing times for NJOY and the original SIGMA-1 method as used in MINX.

The broadened cross sections are written on a new PENDF tape as a series of materials, all with the same MAT number, but each with a different temperature.

Table 3. Comparison of Doppler Broadening in NJOY and MINX

Nuclide	C seconds MINX	(0 to 300 K) NJOY
^{12}C	5.83	0.73
Fe	104.7	31.9
^{235}U	171.1	42.1
^{240}Pu	2239.6	570.1

UNRESR

This module prepares effective self-shielded cross sections versus energy, temperature, and background cross section. The methods used were borrowed from ETOX[7] and are almost identical to those used in MINX except that the accurate Hwang and Henryson quadrature scheme[5] is used. The results are added to the input PENDF tape using a special ENDF/B format (MF=2, MT=152) for use by subsequent modules.

HEATR

The HEATR module computes pointwise prompt heat production cross sections (KERMA factors) and adds them to the PENDF tape using the 300 series of reaction numbers (e.g., MT301 is total heating). The calculation is similar to the MACK code[8] except that photon production is accounted for consistently using an energy-balance method.

Prompt, local heating is a result of the slowing down of charged particles including the recoil nucleus itself. However, ENDF/B does not contain the charged particle spectrum data necessary for the direct calculation. By energy conservation, the energy available for local heating is equal to the total available energy minus the energy carried away by secondary neutrons minus the energy carried away by photons. This approach has the advantage of giving the correct heating for large systems (i.e., few photons escape) when the partition between neutron and photon events is severly misevaluated, or even when photon production is absent.

HEATR computes the average neutron energies directly from ENDF/B angular distributions (MF4) and energy distributions (MF5). Average photon energies are computed from the energies of discrete photons (MF12 and/or MF13) and the energy distributions for continuum photons (MF15). Cross sections are obtained from the PENDF tape.

As shown in Fig. 2, the data produced by HEATR is only one component of the data required for a complete heating calculation. Once the neutron flux has been computed, the heat production cross section from HEATR is used to compute the "prompt local heating," the photon production matrix (see GROUPR) is used to compute the prompt part of the photon source, and the activation cross sections are used to produce the delayed photon precursors. The total photon source is used in a transport calculation to determine the photon flux. This flux is then used with the photon heat production cross section (see GAMINR) to compute the "non-local heating." The last component is the "delayed local heating" due to particle decay of the activation products or fission products. A future NJOY module will provide the data for the decay branch in Fig. 2 directly from ENDF/B-V file 8.

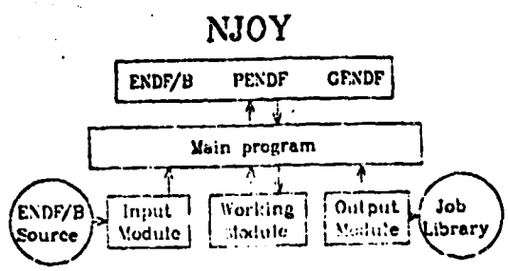

Fig. 1. Overall structure of the NJOY system.

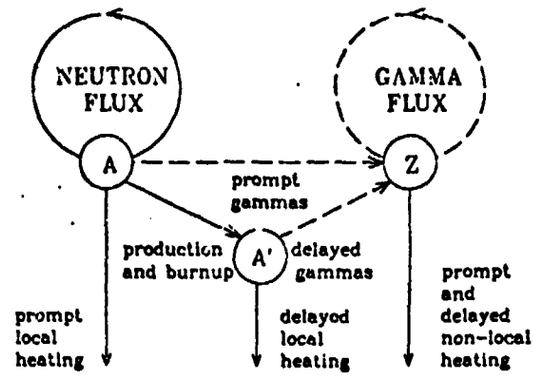

Fig. 2. Procedure for a complete nuclear heating calculation.

THERMR

THERMR is used to generate pointwise cross sections and energy-to-energy scattering matrices in the thermal range. The results are added to the PENDF tape for use by subsequent modules.

Incoherent energy-to-energy P_n or angular scattering matrices can be generated for free scatterers or for bound scatterers when ENDF/B scattering functions are available.[9] The secondary energy grid is determined adaptively for each incident energy and angle or Legendre moment so that linear interpolation is accurate to with a specified tolerance. The incident energy grid is fixed. The incoherent cross section is determined by integrating over these distributions and transferring them onto the grid of the PENDF tape by Langrangian interpolation. Finally, the energy-and-angle distributions are normalized and written onto the PENDF tape

using a modified version of File 6. This approach is more direct than that of FLANGE-II,[10] and it permits multigroup averages to be taken (see GROUPR).

Coherent scattering for hexagonal lattices is handled as in the HEXSCAT code[11] except that more Legendre orders are allowed, and a new approximation is used at high energies where reciprocal lattice shells become closely spaced. In addition, the energy grid is determined adaptively so as to represent the P_n cross sections to within a specified tolerance using linear interpolation. The results are written on File 3 using special MT numbers.

GROUPR

GROUPR is used to produce multigroup cross sections, anisotropic group-to-group neutron scattering matrices, and anisotropic photon production matrices. Special features are provided for ratio quantities (e.g., ν, $\bar{\mu}$, ξ, or photon yields), delayed neutron spectra by time group, and anisotropic thermal neutron scattering. Fission is represented as group-to-group matrices for full generality. All cross sections and matrices can be temperature dependent and self-shielded.

It has been found that all these varied types of data can be processed efficiently and compactly using the following generalized integral over incident energy in group g:

$$\sigma_g = \frac{\int_g F\,\sigma\,\phi\,dE}{\int_g \sigma\,\phi\,dE} \quad , \tag{1}$$

where ϕ is the model neutron flux, σ is a particular cross section, and F is a function which varies for different data types. For example, $\sigma = \sigma_f$ and $F = \nu$ gives the fission neutron production cross section. Matrices for two-body scattering reactions are obtained with

$$F = \int_{g'} f^{CM}(E,\omega)\; P_n\;[\mu(\omega)]\,dW \quad , \tag{2}$$

where f is the angular distribution in the center-of-mass frame, P_n is a Legendre polynomial, ω is the LAB cosine, μ is the CM cosine, and the integration is over all ω that lead to secondary energies in group g'. (GROUPR uses an accurate Gaussian quadrature for this integral). Similarly, continuum scattering uses

$$F = f_n^{LAB}(E) \int_{g'} g(E'\rightarrow E)\,dE' \quad , \tag{3}$$

where g is the secondary energy distribution for the reaction (g may be a delta function for discrete photons).

Thermal coherent reactions are processed as cross sections but incoherent scattering requires special methods because of the relatively coarse incident energy grid. The feature of this reaction is a peak which moves in the (E,E') plane but whose shape changes slowly. Straightforward interpolation along E and E' would lead to double-humped shapes. Therefore, when E is between E_i and E_{i+1}, GROUPR projects up from E_i and down from E_{i+1} along the lines E=E' and adds to get the effective shape at E. Then

$$F = \int_{g'} g_n(E \leftarrow E')dE' \quad , \tag{4}$$

where g_n is the projected distribution.

The incident energy integrals of Eq. (1) are particularly simple. Because of the linearization of the point cross sections on the PENDF tape (see RECONR), trapazoidal integration can be used for all cases except Eq. (2). In that case, the additional structure in F(E) is approximately an oscillatory polynomial of known order which can be accurately integrated by a Gaussian quadrature.

The use of such simple quadrature schemes lends itself to doing many integrations in parallel, thus saving the time required to page the complex cross-section tabulations through memory. NJOY does the incident energy integrations for all secondary groups, all Legendre orders, and all σ_0 values simultaneously. The savings of computing time are illustrated in Table 4.

Table 4. Comparison of Multigroup Calculations Using MINX and NJOY

Test	MINX	NJOY
^{235}U selected cross sections	25.0	5.75
^{235}U P_3 elastic matrix	33.4	4.99
^{235}U P_3 total matrix	567.	21.4
Fe P_3 elastic matrix	58.5	13.8

This parallel processing also insures that all neutron induced cross sections are consistent in precision, weight function, and content, thereby avoiding many of the problems encountered when building coupled sets with neutron data from MINX, photon production from LAPHANO,[12] and heating from MACK.

GROUPR normally uses a model flux appropriate for large systems in the narrow resonance approximation

$$\phi(E) = \frac{W(E)}{\sigma_0 + \sigma_t(E)} \quad , \tag{5}$$

where W is a smooth weight function selected by the user, σ_t is the total cross section, and σ_0 is the background cross section parameter. For thermal reactor problems, where the narrow resonance approximation breaks down, GROUPR can compute the flux appropriate to a heaby absorber mixed with a light scatterer using

$$[\sigma_0 + \sigma_t(E)]\phi(E) = \sigma_0 W\ E) + \int_E^{E/\alpha} \frac{\sigma_s(E')\phi(E')}{(1-\alpha)E'} \quad , \tag{6}$$

where σ_s is the scattering cross section of the absorber and α is the maximum lethargy change in scattering. The integral equation is solved by iteration using the PENDF cross sections. The result is a very accurate accounting of all wide and intermediate resonance effects on self-shielding.

The GROUPR results are written onto the ENDF-like GENDF tape for eventual use by the formatting modules (DTFR, CCCCR, MATXSR).

GAMINR

GAMINR produces photon interaction multigroup cross sections and group-to-group photon scattering matrices from ENDF/B data. Total, coherent, incoherent, pair production, and photoelectric cross sections can be averaged using specified group structure and weight function. The Legendre components of the coherent and incoherent scattering cross sections are calculated using the form factors[13] now available in ENDF/B-IV. These form factors account for the binding of the electron in its atom. Consequently, the cross sections are accurate for energies as low as 1 keV. GAMINR also computes the photon heat production cross section. The resulting multigroup constants are written on a GENDF tape for use by the formatting modules (see MATXSR).

Calculational methods are very similar to those in GROUPR except that special methods had to be developed for doing the integrals required to define the F functions for coherent and incoherent scattering.

GAMINR has many advantages over the older GAMLEG code[14] including P_n coherent matrices, the form factors, and the heat production cross sections. Variable-dimensioning allows very large problems to be run. However, GAMINR is slower than GAMLEG.

ERRORR

This module produces cross section covariances from ENDF/B error files.[15] The current version processes only File 33 (cross sections). This is sufficient to compute covariance between the cross section of group g for reaction χ and group g' for reaction χ' when resonances are not important. The necessary multigroup cross sections can be obtained from a preprocessed supergroup library or generated internally in ERRORR using the methods of GROUPR. The code also has a very general method for constructing covariance matrices for reactions which are linear combinations of other reactions.

As with the other multigroup modules of NJOY, ERRORR writes its results on a GENDF tape for later use by the formatting modules.

The capabilities of ERRORR are very similar to those of PUFF[16] which is based on MINX.

DTFR

This is a formatting module which converts multigroup data from a GENDF tape into a form compatible with transport codes such as DTF[17] and ANISN.[18] Tables can be produced for nn, nγ, and $\gamma\gamma$ data with as many Legendre orders as desired and with up to 100 groups. Thermal data (see THERMR) can be substituted for the normal static data in the low energy groups. Upscatter is allowed, and consistent table truncation is performed for both upscatter and downscatter groups which lie outside the limits of the table. Activity edits can be added to the P_0 tables. Since the edits can be any linear combination of cross sections on the GOUT tape, complex things like gas production are easy to construct. In addition, DTFR makes plots of the multigroup cross sections overlaid on the pointwise data, and it makes isometric plots of the group-to-group matrices (see Fig. 3).

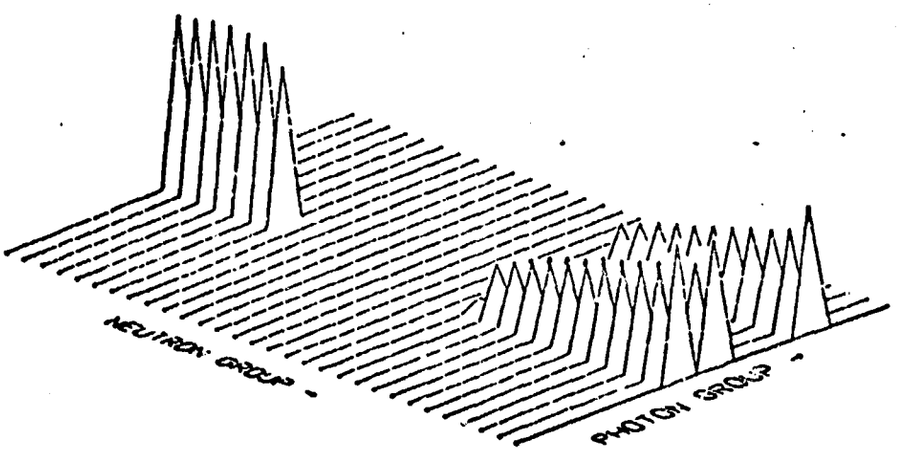

Fig. 3. Photon production matrix for ^{12}C from ENDF/B-IV (30 neutron and 12 photon groups).

CCCCR

The CCCCR module formats GOUT cross sections into interface formats developed by the Committee for Computer Code Coordination (CCCC). Three CCCC-III files[19] are supported.

ISOTXS is a material-ordered file containing cross sections (total, transport, n2n, nα, nd, nt) and P_n scattering matrices (total, elastic, inelastic, n2n).

BRKOXS is a file of shielding factors by temperature and σ_0 (total, transport, capture, fission) and a few auxiliary cross sections used in shielding calculations (e.g., elastic, inelastic, σ_p, ξ).

DLAYXS is a file of delayed neutron yields and spectra by time group. ENDF/B uses the traditional six groups.

Complex data management schemes are used that make it possible to use very large group structures. The conventions used to load these files are the same as those used for the MINX libraries[20] except for a more sophisticated definition for the transport cross section and the treatment of fission. The average fission χ vector is computed by collapsing the GROUPR fission matrix with the multigroup model flux and including delayed contributions.

MATXSR

This module reformats multigroup constants from the GENDF tape into the MATXS interface format. MATXS is a new flexible and comprehensive CCCC-type format designed to hold all the data types which can be produced by NJOY.

The current CCCC cross section files (ISOTXS, BRKOXS, DLAYXS, ISONGX) are rather inflexible. For example, there is no place in ISOTXS for heat production, gas production, or important high threshold reactions like n3n and nαt. Sensitivity studies require partial matrices which are not allowed for. There is no provisions for self-shielding of elastic removal, heat production, or photon production, Furthermore, every data type has a different format, leading to complex and bulky utilities.

MATXS, on the otherhand, has a very general organization designed to hold arbitrary vectors and matrices. The file is first divided into "data types" such as neutron scattering, photon production, gamma scattering, and neutron thermal data. Each type is assigned a name (NSCAT, NGAMA, GSCAT, NTHERM) and new types are easily added. Data types are distinguished by the choice of incident and secondary group structures. In addition to simple cases like n→n or n→γ, MATXS allows for complex coupled sets such as nγ→nγ or n→nγβ.

Each data type is divided into materials specified by nuclide, temperature, and background cross section. Each material is further subdivided

into "vector partials" and "matrix partials." These reaction partials are labeled with Hollerith names so there is no limit on the quantities that can be stored. Vectors are packed with leading and trailing zeroes removed, and matrices are banded as in ISOTXS.

MATXSR reads reactions from the GENDF tape, assigns the Hollerith names, and packs the cross sections into MATXS format. A readable listing of the file is produced if desired, and an index of all the data types, materials, and reactions on the file is printed.

Codes that use MATXS are under development at both Los Alamos and Oak Ridge. One example is TRANSX, an interface to transport codes such as ANISN. TRANSX constructs tables in various formats for $n \rightarrow n$, $\gamma \rightarrow \gamma$, or $n\gamma \rightarrow n\gamma$ coupled sets. The results can be direct or adjoint, material-ordered or group-ordered, prompt or infinite-time, and transport corrected if desired. The code will collapse to a subset group structure, form mixes, and form activity edits which are any linear combination of vectors from MATXS. Upscatter is allowed and thermal cross sections can be used at low energies. Temperature and σ_0 interpolation are included for self-shielding.

CONCLUSIONS

NJOY is a single nuclear cross-section processing system which performs all the functions of MINX, LAPHANO, GAMLEG, MACK, PUFF, FLANGE-II, and HEXSCAT simply and conveniently. It currently processes all ENDF/B-IV and V data types except MF8 (decay data) and MF32 (resonance covariances) and makes the results available to subsequent codes using comprehensive and efficient formats.

REFERENCES

1. D. Garber, C. Dunford, and S. Pearlstein, "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," Brookhaven National Laboratory report BNL-NCS-50496 (ENDF 102) (1975).

2. C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, and R. B. Kidman, "MINX: A Multigroup Interpretation of Nuclear X-Sections from ENDF/B," Los Alamos Scientific Laboratory report LA-6486-MS (1974).

3. O. Ozer, "RESEND: A Program to Preprocess ENDF/B Materials with Resonance Files into a Pointwise Form," Brookhaven National Laboratory report BNL-17134 (1972).

4. P. Rose, Brookhaven National Laboratory, private communication (1975).

5. R. N. Hwang and H. Henryson, II, "Critical Examination of Low-Order Quadratures for Statistical Integrations," Trans. Am. Nucl. Soc. 22, 712 (1975).

6. D. E. Cullen and C. R. Weisbin, Exact Doppler Broadening of Tabulated Cross Sections," Nucl. Sci. Eng. 60, 199 (1976).

7. R. E. Schenter, J. L. Baker, and R. B. Kidman, "ETOX, A Code to Calculate Group Constants for Nuclear Reactor Calculations," Battelle Northwest Laboratory report BNWL-1002 (ENDF-127) (1969).

8. M. A. Abdou, C. W. Maynard, and R. Q. Wright, "MACK: A Computer Program to Calculate Neutron Energy Release Parameters (Fluence-to-Kerma Factors) and Multigroup Neutron Reaction Cross Sections from Nuclear Data in ENDF Format, Oak Ridge National Laboratory report ORNL-TM-3994 (1973).

9. J. U. Koppel and D. H. Houston, "Reference Manual for ENDF Thermal Neutron Scattering Data," General Atomic Co. report GA-8774 (1968).

10. H. C. Honeck and D. R. Finch, "FLANGE-II (Version 71-1), A Code to Process Thermal Neutron Data from an ENDF/B Tape," E. I. DuPont de Nemours and Co. Savannah River Laboratory report DP-1278 (1971).

11. Y. D. Naliboff and J. U. Koppel, "HEXSCAT, Coherent Elastic Scattering of Neutrons by Hexagonal Lattices," General Atomic Co. report GA-6026 (1964).

12. D. J. Dudziak, R. E. Seamon, and D. V. Susco, "LAPHANO: A Multigroup Photon-Production Matrix and Source Code for ENDF," Los Alamos Scientific Laboratory report LA-4750-MS (ENDF-156) (1967).

13. 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," J. Phys. Chem. Ref. Data 4, 471 (1975).

14. K. D. Lathrop, "GAMLEG - A FORTRAN Code to Produce Multigroup Cross Sections for Photon Transport Calculations," Los Alamos Scientific Laboratory report LA-3267 (1965).

15. F. G. Perey, "The Data Covariance Files for ENDF/B-V," Oak Ridge National Laboratory report ORNL-TM-5938 (ENDF-249) (1977).

16. C. R. Weisbin, E. M. Oblow, J. [illegible]ing, J. E. White, R. Q. Wright, and J. Drischler, "Cross Section and Method Uncertainties: The Application of Sensitivity Analysis to Study Their Relationship in Radiation Transport Benchmark Problem," Oak Ridge National Laboratory report ORNL-TM-4847 (ENDF-218) (1975).

17. K. D. Lathrop, "DTF-IV, A FORTRAN Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," Los Alamos Scientific Laboratory report LA-3373 (1965).

18. W. W. Engle, Jr., "A User's Manual for ANISN: A One Dimension Discrete Ordinates Transport Code with Anisotropic Scattering," Union Carbide Corporation report K-1693 (1967).

19. B. M. Carmichael, "Standard Interface Files and Procedures for Reactor Physics Codes, Version III," Los Alamos Scientific Laboratory report LA-5486-MS (1974).

20. R. B. Kidman and R. E. MacFarlane, "LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations," Los Alamos Scientific Laboratory report LA-6260-MS (1976).