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SMR/1220-21

Workshop on

Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

13 March - 14 April 2000

Miramare - Trieste, Italy

Understanding NJOY

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Understanding NJOY

The NJOY Nuclear Data Processing System is used to convert evaluated nuclear data in ENDF format into forms useful for applications. As a bridge between physics and engineering, it is best used by people with some knowledge of things like nuclear reaction theory, resonance theory, or scattering theory on one side, and some knowledge of things like particle transport codes, reactor core calculations, or radiation medicine on the other. In this short course, we will introduce you to the NJOY system, give you a quick outline of the physics of nuclear data, and show you how some of the main applications in nuclear technology link to NJOY results.

Understanding NJOY uses online web pages to introduce you to the subject of nuclear data processing. Normally, you can just follow the NEXT links. To browse through the pages in other orders, use the INDEX links.

If you have an operating version of NJOY 97 and the appropriate data files, you can work through a set of EXERCISES designed to illustrate some of the important features of the code. To do the exercises in order, just follow the NEXT links. To browse through the pages in other orders, use the INDEX links.

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ENDF, NJOY, and Applications

The ENDF formats were originally developed for use in the US national nuclear data files called ENDF/B (the Evaluated Nuclear Data Files). These files went through various versions with names like ENDF/B-III, ENDF/B-IV, and ENDF/B-VI, each version adding both improved data and new capabilities for representing nuclear data . The current ENDF-6 format can represent cross sections for neutrons, photons, and charged particles, including particle yields and distributions in angle and energy, for energies up to several hundred MeV, the radioactive decay properties of reaction products, and estimated errors and covariances of the various nuclear parameters. The ENDF format is now widely used around the world, including the JEF files in Europe, the JENDL files in Japan, and the BROND files in Russia. Thus, even though NJOY was originally designed to work with the US ENDF/B libraries, it now provides a universal capability to work with nuclear data libraries all over the world. For more information on the ENDF format, look at the Introduction to the ENDF Format, which is another web-based course similar to this one.

The NJOY Nuclear Data Processing System is a modular computer code designed to read evaluated data in ENDF format, transform the data in various ways, and output the results as libraries designed to be used in various applications. Each module performs a well defined processing task. The modules are essentially independent programs, and they communicate with each other using input and output files, plus a very few common variables.

- **NJOY** directs the flow of data through the other modules and contains a library of common functions and subroutines used by the other modules.
- **RECONR** reconstructs pointwise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes.
- **BROADR** Doppler broadens and thins pointwise cross sections.
- **UNRESR** computes effective self-shielded pointwise cross sections in the unresolved energy range.
- **HEATR** generates pointwise heat production cross sections (KERMA coefficients) and radiation-damage cross sections.
- **THERMR** produces cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range.
- **GROUPR** generates self-shielded multigroup cross sections,

group-to-group scattering matrices, photon-production matrices, and charged-particle cross sections from pointwise input.

- **GAMINR** calculates multigroup photoatomic cross sections, KERMA coefficients, and group-to-group photon scattering matrices.

- **ERRORR** computes multigroup covariance matrices from ENDF uncertainties.

- **COVR** reads the output of ERRORR and performs covariance plotting and output formatting operations.

- **MODER** converts ENDF "tapes" back and forth between ASCII format and the special NJOY blocked-binary format.

- **DTFR** formats multigroup data for transport codes that accept formats based in the DTF-IV code.

- **CCCCR** formats multigroup data for the CCCC standard interface files ISOTXS, BRKOXS, and DLAYXS.

- **MATXSR** formats multigroup data for the newer MATXS material cross-section interface file, which works with the TRANSX code to make libraries for many particle transport codes.

- **RESXSR** prepares pointwise cross sections in a CCCC-like form for thermal flux calculators.

- **ACER** prepares libraries in ACE format for the Los Alamos continuous-energy Monte Carlo code MCNP.

- **POWR** prepares libraries for the EPRI-CELL and EPRI-CPM codes.

- **WIMSR** prepares libraries for the thermal reactor assembly codes WIMS-D and WIMS-E.

- **PLOTR** reads ENDF-format files and prepares plots of cross sections or perspective views of distributions for output using VIEWR.

- **VIEWR** takes the output of PLOTR, or special graphics from HEATR, COVR, DTFR, or ACER, and converts the plots into Postscript format for printing or screen display.

- **MIXR** is used to combine cross sections into elements or other mixtures, mainly for plotting.

- **PURR** generates unresolved-resonance probability tables for use in representing resonance self-shielding effects in the MCNP Monte Carlo

code.

- **LEAPR** generates ENDF scattering-law files (File 7) for moderator materials in the thermal range. These scattering-law files can be used by THERMR to produce the corresponding cross sections.

- **GASPR** generates gas-production cross sections in pointwise format from basic reaction data in an ENDF evaluation. These results can be converted to multigroup form using GROUPR, passed to ACER, or displayed using PLOTR.

More details on all of these modules will be found on subsequent pages--just keep pressing NEXT, or to browse through the pages in other orders, use the INDEX links.

Note that some of these modules do calculations to transform the evaluated nuclear data, and others format the results of the calculations for various nuclear applications. One very basic application is the multigroup particle transport code, which is used to compute neutron and photon fluxes and reaction rates for reactor design, shielding and radiation protection, criticality safety, experimental facility design, medical applications, and so on. Familiar examples of such codes include ANISN from Oak Ridge and the "DANT" series from Los Alamos. NJOY can prepare data for these codes through several paths, including DTFR, CCCCR, and MATXSR. These days, people are making more and more use of the powerful Monte Carlo method, which uses very detailed and faithful representations of complex problems. Data for the popular MCNP code can be produced with ACER. For direct thermal-reactor core calculations, the WIMS code series from Great Britain is very widely used, and NJOY's WIMSR module can produce the appropriate libraries for it. The modular structure of NJOY lends itself to adding additional applications without having to reinvent the core transformations that NJOY does to evaluated nuclear data.

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NJOY Data Flow

NJOY uses a data-flow model to process evaluated nuclear data. Each module reads some data from one or more input files, transforms it, and writes the results on one or more output files. The order that the modules are used and the particular input and output files used are specified as in the following example:

```
[copy an ENDF file onto "tape20"]

reconr
20 21
  ...specific input for RECONR...
broadr
20 21 22
  ...specific input for BROADR...
groupr
20 22 0 23
  ...specific input for GROUPR...
dftr
23 24 22 25
  ...specific input for DTFR...
stop

[copy tape24 to the DTF library]
```

In this case, RECONR reads the original ENDF tape and reconstructs the resonances and nonlinear interpolation schemes to prepare a PENDF (pointwise ENDF) tape on unit 21. BROADR reads the PENDF tape, Doppler broadens the pointwise cross sections, and writes a new temperature-dependent PENDF tape on unit 22. Sometimes it needs some data from the ENDF tape, and this is why `tape20` is also provided as input. Next, the information from the ENDF and PENDF tapes is run through the multigroup averaging process and written in GENDF format (a special groupwise variation of the ENDF format) on `tape23`. Finally, the multigroup constants on `tape23` are converted to DTF format on `tape24`. The PENDF input for DTFR is used for the plots, which appear on `tape25`.

All NJOY jobs are variations of this basic data-flow structure. I/O units with numbers from 20 up can be used to couple the modules together, for the original input files, or for output files. NJOY always names these "tape20", "tape21", and so on. Units from 10 to 19 are used as scratch files. They may be named as tapes, or have special system names. Units with numbers below 10 are used for system input and output files, such as "output".

NJOY is normally run under the control of some kind of system shell. For unix, the NJOY input commands go into the standard input, and runtime messages go out on the standard output. Therefore, if the input "deck" (such as the one outlined above) is named "inx", the following would cause a normal NJOY run to execute:

```
njoy < inx
```

The short listing containing progress messages, notes, and error messages would appear on the screen (or it could be redirected to a file, *e.g.*, `outx`), and the full listing would appear on a file named "output".

Please don't be shocked at our pleasure in using the terms "tape" and "deck." Later, you will find us talking about input "cards." We do this out of respect for the history of computing, and because we can still remember using tapes and decks of cards!

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PENDF and GENDF

The data-flow example on the previous page introduces the terms "PENDF tape" and "GENDF tape." Because these files will be very important for all the NJOY examples, we define them more completely here:

- **PENDF tape:** a pointwise version of an ENDF tape where any resonance parameters or nonlinear interpolation ranges have been converted into pointwise cross sections suitable for linear interpolation to within specified accuracy criteria. The File 1 comments have been simplified, although the directory is correct. Resonance parameters have been removed from File 2. Only Files 3, 6 (for thermal data only), and 13 are given for data; the other information, such as angle and energy distributions, must be read from the corresponding ENDF tape. Multiple temperatures may be given for a material by repeating each "MAT" in order of increasing temperature.

- **GENDF tape:** a multigroup version of an ENDF tape with the group structures, temperatures, and background cross section defined in File 1, "vector" cross sections given in File 3, and group-to-group matrices given in File 6. Higher MF Files are used for photons and charged particles.

Using these standardized files supports the modular nature of NJOY. Different modules can sometimes be run in different orders and combined in various ways. Internally, all NJOY modules use a common set of subroutines for reading and writing the ENDF, PENDF, and GENDF "tapes" (they are located in the NJOY module).

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Formatted and Binary Modes

ENDF tapes received from a distribution point, be they ENDF/B, JEF, JENDL, CENDL, or BROND, come in a formatted ASCII mode that can be easily read or printed. However, this is not the most efficient form to use for communicating between different processing modules in NJOY. Binary files are much more efficient because it is not necessary to repeatedly convert the data between the binary forms used in memory and the ASCII forms.

Although the ENDF format specifies a standard binary mode, NJOY uses a special blocked-binary mode that divides each ENDF "record" into one or more blocks of data of bounded size. The NJOY subroutines that read and write ENDF records know how to handle the binary mode and how to convert back and forth between binary and ASCII. NJOY normally uses a page size of 326 words for these binary blocks, which is small enough to use conveniently and large enough to reduce the total number of I/O operations to a reasonable value.

NJOY contains a special module called MODER for converting back and forth between the ASCII and binary forms. It uses negative unit numbers to indicate binary files. Therefore, the previous example of NJOY data flow would like like this when using binary mode:

```
[copy an ENDF file onto "tape20"]

moder
20 -21
reconr
-21 -22
  ...specific input for RECONR...
broadr
-21 -22 -23
  ...specific input for BROADR...
groupr
-21 -23 0 -24
  ...specific input for GROUPR...
dftr
-24 25 -23 26
  ...specific input for DTFR...
stop

[copy tape25 to the DTF library]
```

MODER also has other capabilities. See the MODER Input Instructions.

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NJOY Input

Beginning with NJOY97, the standard Fortran "read *" method is used to read input quantities and strings. Earlier versions used a home-grown scheme with similar properties. The main difference between these two approaches is that the new one delimits string data with single quote characters, but the old one used star characters.

All input is free form, and different quantities can be separated with spaces or commas. Numerical quantities can be given with or without decimals, and "E" or "e" can be used for scientific notation. String input consisting of single words that start with an alphabetic character do not require delimiters. Longer strings with spaces and special characters must be surrounded by single quote characters.

Lines of input for NJOY are often organized so that the parameters at the ends of the lines have default values. Therefore, you can often stop giving numbers before the entire I/O list is exhausted by using the slash (/), or division sign, character. Some examples follow:

```
1    reconr
2    20 21
3    1395 1/
4    .01/
5    '92-U-235'/
```

Line 1 is a string value that doesn't require delimiters. Line 2 is a line with only two values in the I/O list, and both are given. No terminating / is required. Line 3 is a line with three items in the I/O list. The last variable, namely `ngrid`, will take its default value of 0. Line 4 has 4 values, and the last three will all be defaulted. The value .01 could also be written as 1e-2 or 1.0e-2. Line 5 has only one value, which is a string. Since the string has spaces and starts with a digit, it has to be delimited with quote characters. Any line that consists of string data must end with the / character.

The NJOY97 test problems provide numerous examples of the input syntax.

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RECONR: Linearization and Resonance Reconstruction

Most NJOY processing sequences start with RECONR. It fills two roles. First, it goes through all the reactions included on the ENDF tape and chooses a union grid that allows all cross sections to be represented using linear interpolation to a specified accuracy. This step removes any nonlinear interpolation ranges (*e.g.*, log-log, linear-log). It also makes it possible for all summation reactions to be reconstructed as the sum of their parts (*e.g.*, total, total inelastic, total fission). Second, for resonance materials, it reconstructs the resonance cross sections (elastic, fission, capture) on a union grid that allows them all to be represented within certain accuracy criteria, and then combines the resonance data with the other linearized and unionized cross sections. The results are written in PENDF format.

RECONR is fairly easy to use. Issues that deserve more discussion include:

- Linearizarization and Unionization - how are the energy grids chosen?
- Resonance Reconstruction - what options are available?
- Integral Thinning - practical libraries *vs* full accuracy.
- Numerical Precision - how many significant figures are used to represent energies and cross sections?
- Unresolved Treatment - how does RECONR interact with UNRESR and PURR?

They will be discussed on the pages to follow.

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Linearization and Unionization

All ENDF-format evaluations define their cross sections over at least part of the energy range using tabulations. In many cases, part of some of these tabulations specify that a nonlinear interpolation scheme is to be used to obtain intermediate values. NJOY wants to get everything in linear form for several reasons:

- the method used for Doppler broadening requires linearly interpolated piece-wise functions;
- the ACE files for use with MCNP require linear-linear functions;
- linear functions are easy to average into multigroup form;
- linear functions are easy to plot; and
- summation cross sections, such as the total cross section, total inelastic, or total fission, cannot be properly defined as the sum of their parts except when given as linear.

The classic example of the last point is the thermal energy range, where the zero-degree elastic cross section is usually constant with energy (and uses linear-linear interpolation), but the radiative capture cross section follows a $1/v$ law and uses log-log interpolation. There is no simple "graph-paper" interpolation scheme that can represent the sum of the elastic and capture cross sections to the same accuracy as the original parts. However, if both the elastic and the capture are linearized to a given accuracy on the same "union grid," their sum is also linearized to the same accuracy on this grid.

RECONR solves this problem as follows. It first skips the total cross section and goes to the elastic cross section (MF=3, MT=2). It starts with a list of "nodes" that may include energy values given by the user, may include energies derived from the resonance parameters, and certainly includes the thermal value .0253 eV. It then adds in any energy points given in the elastic section of File 3, and if necessary, it adds in points on the 1, 2, 5, 10, ... grid for each energy decade. Now it looks at each "panel" described by a pair of these nodes and decides whether to divide the panel in half. It will divide the panel if the energy step is too large to represent the $1/v$ function to within the specified accuracy, or if the interpolation scheme is nonlinear, it will divide the panel if the difference between the specified interpolated function and the linear interpolate is too large. It continues subdividing and checking until the desired accuracy has been achieved over the entire energy range.

The reason for checking the $1/v$ accuracy for elastic scattering is that Doppler broadening tends to add a $1/v$ component to the elastic cross section, and this grid will help to handle that correctly in BROADR, even when the radiative capture reaction is missing or extraordinarily small.

Once the elastic cross section has been linearized, the code moves on to the next reaction, perhaps (n,2n), and determines whether any additional points have to be inserted in the union grid to represent that reaction to within the desired tolerance. RECONR continues in this way until all the reactions have been checked. The result is therefore a union grid able to represent all the cross sections with linear interpolation, and that implies that it can also represent the sums of those cross sections with the same accuracy.

The following input deck will carry out the linearization and unionization process for H-1 from ENDF/V-VI (assuming that the appropriate ENDF file has been mounted on unit 20):

```
reconr
20 21
'1-H-1 from ENDF/B-VI'/
125 1/
.01/ 1% linearization
'1-H-1 from ENDF/B-VI'/
0/
stop
```

For a complete description of these input lines, see the RECONR Input Instructions. *HINT: use the right-hand button on your browser to bring the link up in a separate window. You can then view the input example and the input instructions at the same time.* An examination of the sections of File 3 for MT=1, 2, and 102 will illustrate the kind of energy grids produced and the unionization. Note that the standard .0253 eV value and energies on the 1, 2, 5, 10, 20, ... sequence were included.

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RECONR:
Resonance Reconstruction

ENDF-format files for the lighter nuclides usually represent the entire cross section using tabulated values. However, as the target mass increases, more and more resonances occur for reactions like elastic scattering, radiative capture, and fission. The number of energy grid points required to represent the function in tabulated form becomes excessive. At this point, the evaluators start to use resonance parameters to represent all or part of the cross section over a range of energies called the "resonance range."

The resonance range may consist entirely of resolved resonances, or there may be both resolved and unresolved ranges. We will discuss the unresolved part later. The resolved range usually starts at 1e-5 eV, or some other low energy (such as 1 eV) and extends until the resonance effects are small, or until a changeover to the unresolved representation occurs. The resonance parameters are given in File 2 with MT=151. For a more detailed description of the ENDF resonance formats, see our Introduction to the ENDF Formats. The cross sections in File 3 over the resolved range are usually zero, but in some cases, there may be small "background" cross sections that are to be added to the cross sections computed from the resonance parameters to correct for problems (such as the inadequancy of a single-level Breit-Wigner representation). ENDF provides discontinuities represented as double energy points at the ends of the resonance ranges. These regions of background cross section often confuse people who look at File 3 in ENDF evaluations and ask, "Why is the cross section zero? That can't be right!"

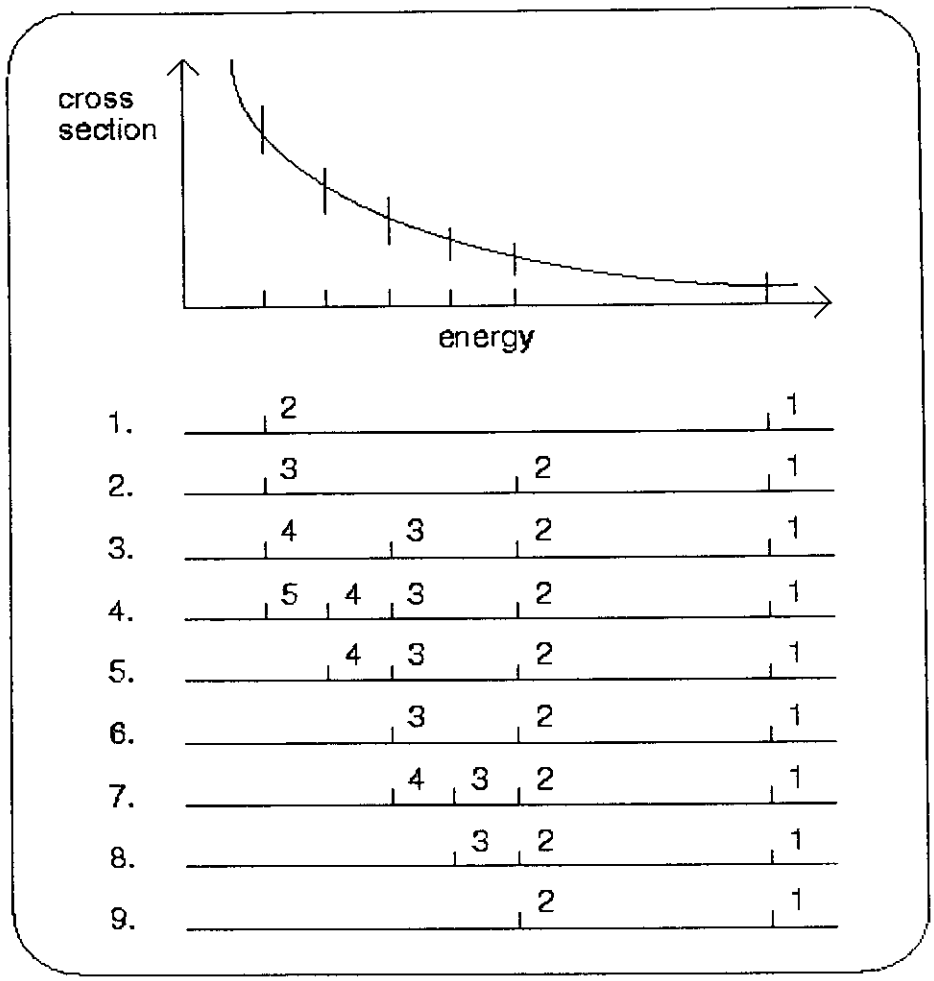
The ENDF format provides several options for representing resonance parameters. The most commonly used are

- Single-Level Breit-Wigner - simple and easy to use, but not always as accurate as needed (can produce negative cross sections),
- Multi-Level Breit-Wigner - gets rid of the negative cross sections, but much more expensive to use. Can't represent multichannel effects that are sometimes important.
- Reich-Moore - very faithful for all but the lightest nuclides. It is becoming the preferred representation for important materials.

Except for run time and negative cross sections, the representation used is transparent to the RECONR user.

RECONR reads in the resonance parameters, and it adds the resonance energies and the half-height energies to the list of nodes available from the linearization and unionization process. The resonance nodes are truncated to five significant digits. This makes it easier to find them on a PENDF listing, and it prevents them from being thinned away in BROADR. This choice of starting nodes for the resonance reconstruction process assures that no important structures will be missed. The code then works through each panel defined by these nodes, compares the cross section computed at the midpoint with a linearly interpolated value, and decides whether to

add the new midpoint to the grid. This process of halving and checking continues until convergence is achieved over the entire energy range using a special inverted-stack logic that is also used elsewhere in NJOY. The following figure shows the points in the stack at several different stages of the linearization of an energy panel.



Once the resonance energy grid and the resonance cross sections have been determined, RECONR merges them with the linearized and unionized ENDF cross sections, and write the results on an output file in PENDF format.

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RECONR:
Integral Thinning

The criteria used for deciding when to stop halving intervals during resonance reconstruction are complex. Modern resonance evaluations can be very detailed, yielding hundreds of thousands of energy points when fully expanded. These very large tabulations are expensive to produce, to store, and to Doppler broaden or average. However, almost all of the uses of RECONR output result in integrating over the cross sections; this is true for both Doppler broadening and multigroup averaging, and it is also true for all ultimate applications, even continuous-energy Monte Carlo transport calculations. Therefore, if the reconstructed resonance cross sections contain features that cause negligible effect on these integrals, these features can be removed without affecting the ultimate results significantly. This is why RECONR includes an option for carrying out "integral thinning" while it is generating its resonance cross sections.

The main user input to RECONR is the reconstruction tolerance, ERR. It is given as a fractional quantity, *e.g.*, 0.001, to represent 0.1%. The default behavior is to set the auxiliary thinning parameters to standard values ERRMAX=20*ERR and ERRINT=ERR/10000. RECONR will then always halve intervals until the fractional difference between the computed cross sections and the interpolates are less than ERRMAX for all reactions. Once this has been achieved for an interval, it will check to see how much the panel will change the resonance intergal. If the change is smaller than ERRINT, the subdivision process will be terminated. When the subdivision terminates, it is possible to make a rough estimate of the effect of the termination on the resonance integral. As an example of this process, here is an example of the output provided by RECONR when processing U-238 from ENDF/B-VI:

```
number of user and resonance nodes = 3834
points in initial unionized grid = 4230
points added by linearization = 215

                estimated maximum error due to
                resonance integral check (errmax,errint)
                and significant figure truncation

  upper       elastic     percent error     capture     percent error
  energy      integral   res-int sig-fig    integral   res-int sig-fig
1.00E-05
1.00E-04      2.15E+01    0.000   0.000      1.86E+02    0.000   0.000
1.00E-03      2.15E+01    0.000   0.000      5.88E+01    0.000   0.000
1.00E-02      2.15E+01    0.000   0.000      1.86E+01    0.000   0.000
1.00E-01      2.15E+01    0.000   0.000      5.91E+00    0.000   0.000
1.00E+00      2.14E+01    0.000   0.000      1.96E+00    0.000   0.000
2.00E+00      6.32E+00    0.000   0.000      3.32E-01    0.000   0.000
5.00E+00      7.90E+00    0.000   0.000      6.29E-01    0.000   0.000
1.00E+01      1.47E+01    0.000   0.000      1.30E+02    0.000   0.000
2.00E+01      5.27E+00    0.000   0.000      6.59E-01    0.000   0.000
5.00E+01      1.02E+02    0.000   0.000      1.09E+02    0.000   0.000
1.00E+02      1.89E+01    0.000   0.000      1.26E+01    0.000   0.000
2.00E+02      5.05E+01    0.000   0.000      1.34E+01    0.000   0.000
5.00E+02      1.93E+01    0.000   0.000      5.14E+00    0.004   0.000
1.00E+03      1.50E+01    0.001   0.000      2.45E+00    0.014   0.000
2.00E+03      1.47E+01    0.002   0.000      1.33E+00    0.042   0.000
5.00E+03      1.77E+01    0.006   0.000      1.09E+00    0.113   0.000
```

```
points added by resonance reconstruction =140468
points affected by resonance integral check =103592
points affected by significant figure reduction =      0
final number of resonance points =144493
number of points in final unionized grid =144913
```

Note that the output shows the elastic and capture integrals over roughly logarithmic energy bands running through the resolved range (1e-5 eV to 5 keV). The "res-int" column shows an estimate of the error made by integral thinning, *e.g.*, a maximum of 0.1% for U-238 capture at high energies. About 100000 points were removed from the final energy grid by the integral check. This is a major savings for a fairly small impact on the least known part of the U-238 cross section.

If this increased error is unacceptable, it can be reduced in two ways: either set ERRMAX closer to ERR, or make ERRINT smaller than ERR/10000.

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RECONR:
Numerical Precision

Standard ENDF-format files use an 11-column field to represent floating-point numbers. In order to maximize the number of significant digits possible within this limit, unnecessary characters are eliminated. Therefore, energies usually take on forms like " 1.234567+3", which provides for 7 significant digits. If larger exponents are needed, the format drops back to 6 or 5 significant digits.

One of the few places that this standard numerical format can be inadequate is for the representation of the cross sections reconstructed for very narrow resonances. Since narrow resonances only occur for a restricted range of energies (say, 1 eV to 1 MeV), 11-column forms such as " 123.456789" can provide an accuracy of 9 significant digits, which is always sufficient in practice.

However, the need for more than 7 sigificant digits is rare. Moreover, the smoothing effect of Doppler broadening usually assures that only 7 digits are needed at 300K, even if 11 are needed at 0K. In addition, we want to preserve as much similarity between PENDF tapes and ENDF tapes as possible. For these reasons, we have adopted a complex system for the precision of energy values used in NJOY97. The initial nodes, the values read from standard ENDF tapes, and values added by RECONR (such as those from the 1, 2, 5, 10, 20, ... sequence) will normally have only a few significant digits (typically 5 or fewer). This helps to identify them on listings, and BROADR will try not to thin out energy values with several zeros on the end. In subdividing energy panels to linearize resonance cross sections, RECONR will first try to fit the actual function with numbers limited to the 7-digit standard form. Only when this is impossible will RECONR resort to the 11-digit form. It is fairly easy to spot such numbers on a listing of the 0K PENDF tape.

In BROADR, the code will preferentially use the numbers with lower numbers of significant digits as nodes in its reconstruction process. Thus, if 11-digit numbers are not needed to represent the Doppler-broadened cross section, the PENDF tape from BROADR will contain only the ENDF-standard 7-digit form, and our goal of maximum compatibility with the appearance of standard ENDF tapes will have been achieved. However, if the more precise 11-digit values are needed to get the specified accuracy, they will be used.

All cross sections are adjusted to fit into the normal ENDF 7 significant-figure format.

NJOY97 binary ENDF tapes use 64-bit representations for all numbers in order to support the scheme described above. The number of significant digits in the binary versions of each number matches the number in the ASCII versions, which helps to preserve consistency between NJOY runs made in binary and ASCII modes.

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RECONR: Unresolved Range

For the heavier nuclei, there is a region above the resolved range where the resonances get so close together that they can no longer be separated. However, there can still be important resonance effects, such as self shielding, active in this "unresolved" range. In ENDF-format evaluations, the unresolved range is represented by giving average resonance widths and spacings and the statistical rules obeyed by these widths and spacings. RECONR converts these statistical representations into actual "infinitely-dilute" cross sections. These are the values appropriate for thin samples or dilute mixtures where resonances don't interfere with each other due to their effects on the neutron flux. The effects of each resonance simply add together in computing the net cross section, and the cross section can be computed by doing weighted averages using the specified probability distributions.

There are some complicated rules used for determining the energy grid in the unresolved range. Modern evaluations normally give the parameters as functions of energy, and the rule is to first compute the cross sections at these energy points, and then to interpolate between the cross sections to get intermediate values. However, some of the older evaluations contain rather large jumps in energy in between the grid values given, *e.g.*, decade steps. The evaluators did not expect that their work would be linearly interpolated across such large steps, because earlier ENDF rules did not require that. Therefore, RECONR watches for large steps, and it automatically subdivides them using points from a standard grid with roughly logarithmic steps. This gives a better approximation of the roughly $1/v$ shapes expected. Some evaluations for minor isotopes that were made without benefit of detailed experimental data just assume that the average resonance parameters are constant across the unresolved range. RECONR automatically subdivides the range using its standard grid, thus yielding a cross section with a reasonable shape resulting from the natural energy dependences in the resonance formulas.

RECONR includes the unresolved contributions in the normal elastic, fission, capture, and total tabulations in File 3 of the PENDF tape. However, it also generates a new section of File 2 with the special value MT=152 that also contains the unresolved cross sections. This section will be overwritten with self-shielded cross sections by the UNRESR module, if it is run. Otherwise, the MT=152 section from RECONR will be available for GROUPR to use while generating multigroup constants.

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BROADR: Doppler Broadening

BROADR adds temperature dependence to the pointwise cross sections generated by the RECONR module (see UNRESR and PURR for temperature dependence in the unresolved energy range). It can also be used to rebroaden the results of a previous BROADR run to a higher temperature.

In a material at temperature T, the target atoms and molecules are moving around randomly with a distribution of velocities given by the Maxwell-Boltzman function:

$$P(\mathbf{v}',T)\,d\mathbf{v}' = \frac{\alpha^{3/2}}{\pi^{3/2}}\exp(-\alpha v'^2)\,d\mathbf{v}' ,$$

where α=M/(2kT). When a neutron moves through the material, it is the *relative velocity* between the neutron and the target nucleus that determines the proper cross section to use. We can define a single effective cross section for neutrons with velocity v by conserving the reaction rate:

$$v\bar{\sigma}(v,T) = \int d\mathbf{v}'\,|\mathbf{v}-\mathbf{v}'|\sigma(|\mathbf{v}-\mathbf{v}'|)P(\mathbf{v}',T)$$

BROADR uses methods based on early versions of Cullen's SIGMA1 code to compute these effective cross sections for linear-linear representations of the basic reaction cross sections. The basic cross sections are obtained from a PENDF tape generated by RECONR or produced in a previous BROADR run. The Doppler-broadened effective cross sections are written out as a multi-temperature PENDF tape.

The following is an example of a simple BROADR run to Doppler broaden the results of a previous RECONR run (on `tape21`) for the H-1 evaluation (on `tape20`):

```
20 21 22
125 1/
.001/
300/
0/
```

To understand this deck, study the input instructions. *Hint: use the right-hand button with your browser to bring the instructions up in a separate window for easy comparison with the lines in the example.*

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BROADR:
Typical Broadened Cross Sections

The effects of temperature on typical cross sections is best illustrated by giving several examples. First, here is the (n,α) cross section for B-10 shown for temperatures of 0K, 3000K, and 3000000K. This shows that a $1/v$ cross section is invariant under Doppler broadening.

Postscript Figure

Next, here is the elastic cross section for carbon shown for temperatures of 0K, 300K, 3000K, and 30000K. This shows that a constant cross section will develop a $1/v$ tail under Doppler broadening.

Postscript Figure

Finally, here is how resonance cross section behave under Doppler broadening. The (n,gamma) cross section for Pu-240 is shown for temperatures of 0K, 30000K, and 300000K. Resonances with energies larger than kT/A broaden symmetrically (and their areas tend to remain constant). Low energy resonances develop an additional $1/v$ tail, and their areas do not remain constant under Doppler broadening.

Postscript Figure

These effects are best understood by noting that Doppler broadening preserves the reaction rate $v*\sigma(v)$, and a finite reaction rate is expected for T larger than zero even as v goes to zero.

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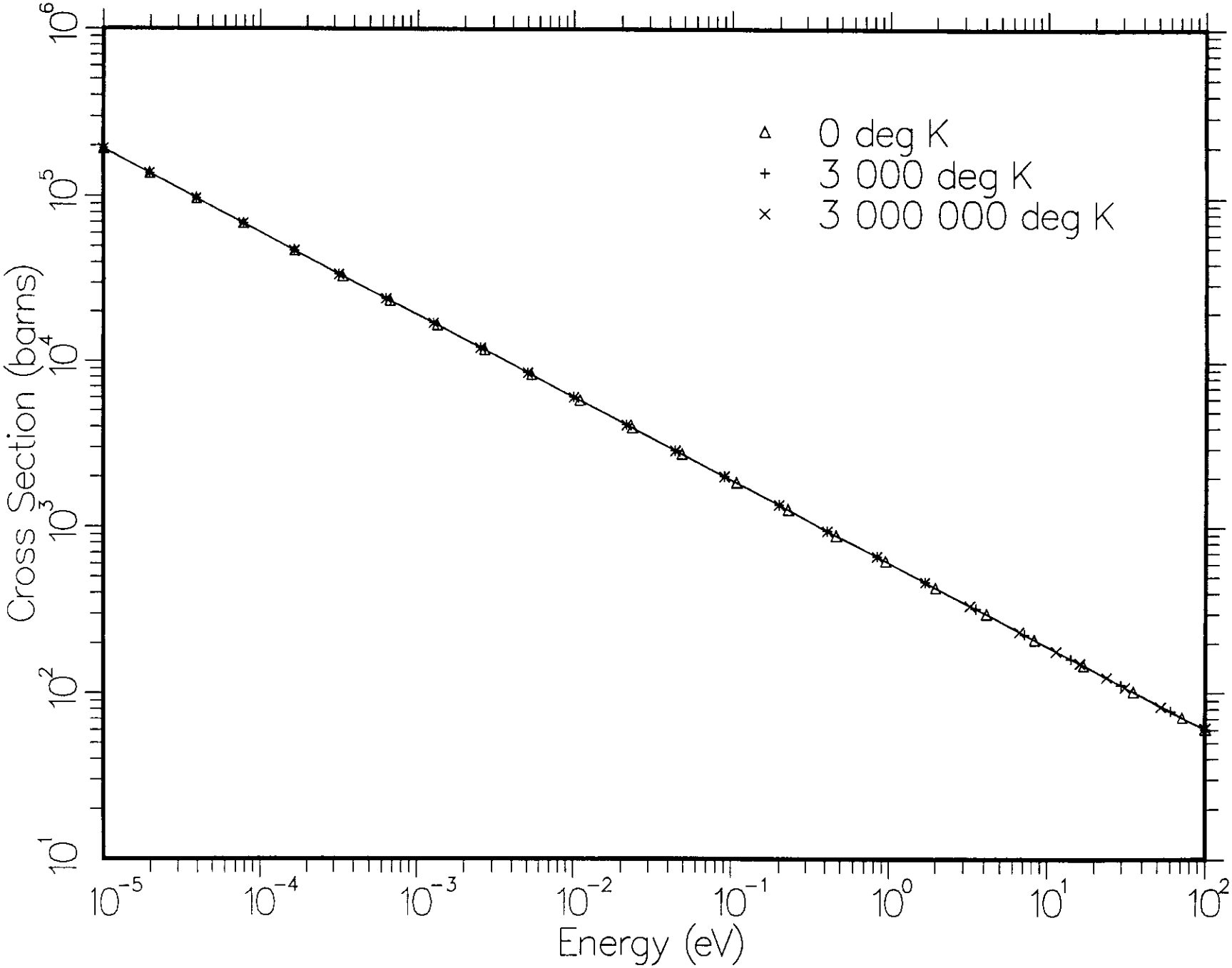
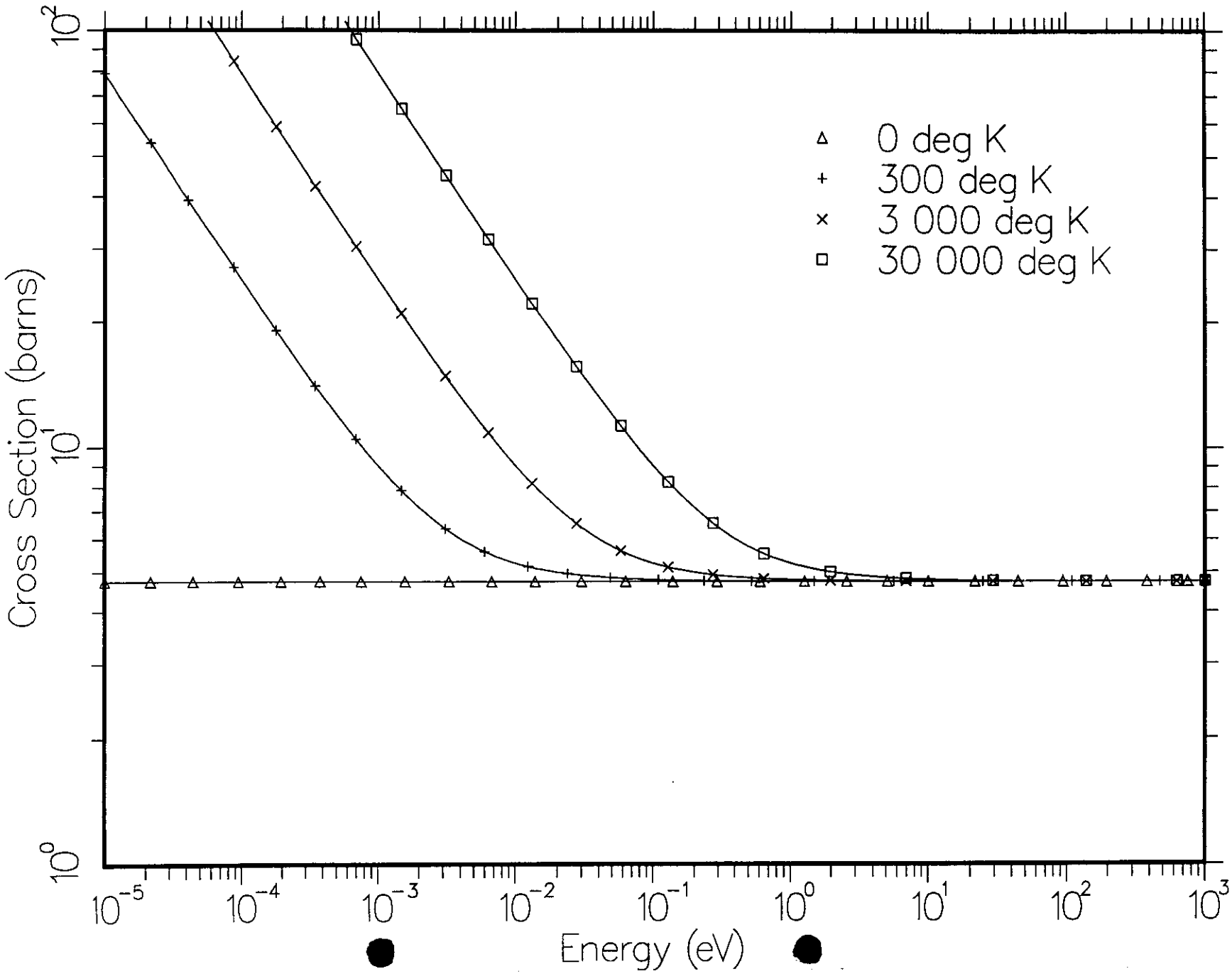

Cross Section (barns)
Energy (eV)
0 deg K
3 000 deg K
3 000 000 deg K
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}


Cross Section (barns)
10^2
10^1
10^0
0 deg K
300 deg K
3 000 deg K
30 000 deg K
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
10^2
10^3
Energy (eV)

Cross Section (barns)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
Energy (eV)
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}

BROADR: Energy Grids

As discussed in the RECONR section, the zero-temperature PENDF tape uses a unionized energy grid that represents the cross sections to within certain accuracy criteria using linear-linear interpolation. As shown on the preceeding page, the shapes of the cross sections can change radically after Doppler broadening, and we should expect that the optimum unionized energy grid will have to change also.

As an example of this, the following graph shows the 20 eV resonance in the (n,γ) cross section of Pu-240 for the two temperatures 0K and 300000K. Note that the broadened curve doesn't need as many energy points near the center of the resonance as the zero-temperature curve, but it needs more points out on the steep sides of the wings of the resonance near 15 eV and 25 eV.

Postscript Figure

BROADR generates the new grid using a method very similar to the one used for resonance reconstruction by RECONR. Starting at one particular energy point, BROADR skips forward over some of the energy points in the input grid to find the top of a "panel" to be relinearized. The top of the panel is determined by trying several criteria, such as a maximum lethargy step, or a maximum number of points skipped. But most important, in NJOY97, BROADR tries to keep energy values that end with several zeros. This means that the original "node" values from RECONR will be kept in the new grid. These include standard values like .02530000, 1.000000+2, 2.000000+2, 5.000000+2, and 1.000000+3. But they also include the center energies of the resonances and the two half-height values used to seed resonance reconstruction. This approach keeps all the convenient simple points, preserves all the important structure, and allows BROADR the most possible freedom for generating an ideal new energy grid within these constraints.

Once the upper and lower limits of the panel have been determined, the code then checks whether it should be divided in half by comparing the computed Doppler-broadened cross section at the midpoint to the linearly interpolated value. It uses the same stack logic, fractional accuracy checks ,and resonance integral checks as RECONR. Of course, all of the broadened reactions are checked at each midpoint, which preserves the union nature of the energy grid.

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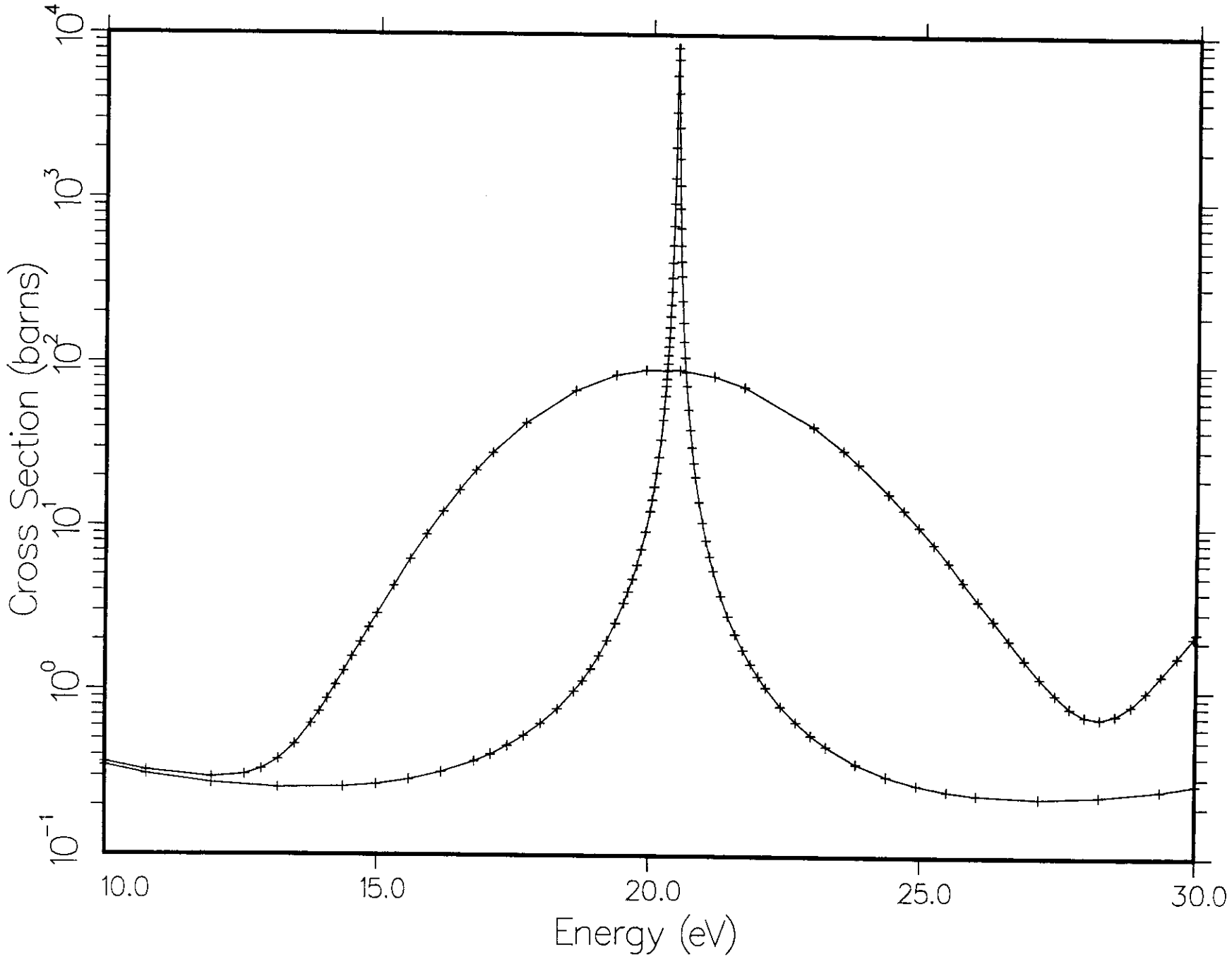
Cross Section (barns)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10.0
15.0
20.0
25.0
30.0
Energy (eV)

BROADR:
Numerical Precision

The energy grid on the input PENDF tape may have been produced by RECONR, or it may be the result of a previous BROADR run. In either case, most of the energy values will be given to seven significant figures using the standard 11-column ENDF format, *e.g.*, 1.234567+1. It is possible that some of the input energies will use the nine-digit form, *e.g.*, 1.23456789. All of the cross section values will use seven significant figures.

When BROADR determines its new union grid, all the "nodes" used as starting points for the relinearization can be represented with the seven-digit form. The new points in the grid are produced just as in RECONR, and it is possible that nine-digit energies may be required in some cases. However, broadening tends to smooth the cross sections, and the nine-digit energies will often disappear. All Doppler-broadened cross sections are reduced to seven significant figures on output.

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BROADR:
Broadenable Reactions

As demonstrated on the preceeding pages, temperature dependence can be introduced by Doppler broadening smooth cross sections at low energies (less than about $16kT/A$). In addition, cross sections with features that are sharp with respect to kT/A, such as resonances, will show temperature dependence. Therefore, the reactions that need to be Doppler broadened are normally elastic, fission, and capture. Sometimes (n,alpha) reactions are present at low energies also. Cross sections in the unresolved resonance range cannot be broadened (see UNRESR and PURR).

The maximum energy for broadening, `thnmax` is defaulted to either the first reaction threshold (typically MT=51, the first inelastic level), the start of the unresolved energy range, or 1 MeV, whichever is the smallest. BROADR selects the set of reactions to be broadened by looking for those that are present in this energy range, which is usually elastic, fission, and capture.

It is possible that these reactions will show no changes under Doppler broadening over much of this energy range. For example, resonances in light isotopes tend to be broad with respect to thermal energies. However, we usually just go ahead and run BROADR on everything.

If you want to use NJOY cross sections for supernova calculations, you may want to include more reactions, such as the first few inelastic levels. There is an option with `thnmax` negative that allows this.

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BROADR: Thermal Quantities and Resonance Integrals

In the thermal reactor business, quite a bit of insight into the behavior of a particular evaluation can be obtained by examining certain thermal cross sections and resonance integrals. In a reactor, most fission neutrons are born from fission reactions at thermal energies. The quantities of interest there are the fission cross section itself, the competing capture cross section, and the number of fission neutrons produced per reaction, nu-bar. The deviation of the shape of the cross sections from a $1/v$ shape is also of interest. The fission neutrons are produced at energies up around 1 MeV, and they have to slow down to thermal energies before producing more neutrons to continue the chain reaction. The quantities of interest here are the fission and capture resonance integrals, which help determine the probability that a neutron will disappear before reaching thermal energies. For these reasons, the following simple parameters have come into wide use:

- fission cross section at thermal
- fission nu-bar at thermal
- capture cross section at thermal
- thermal Maxwellian fission integral
- thermal Maxwellian capture integral
- fission g-factor (deviation from $1/v$)
- capture g-factor
- thermal alpha integral
- thermal eta integral
- thermal K1 integral
- fission resonance integral
- capture resonance integral

The conventional thermal energy is 0.0253 eV. If the cross section has a $1/v$ shape, its integral weighted against a Maxwellian spectrum for 0.0253 eV is given by

$$I = \int \sigma(E)(E/kT)\exp^{-E/kT} d(E/kT)$$

$$I = \int \sigma(kT)\sqrt{kT/E}\,(E/kT)\exp^{-E/kT} d(E/kT) = \frac{\sqrt{\pi}}{2}\sigma(kT)$$

$$G = \frac{2}{\sqrt{\pi}}\frac{I}{\sigma(kT)}$$

where the factor G provides a measure of the deviation from a $1/v$ shape. It will be unity for a pure $1/v$. Similarly, the alpha, eta, and K1 integrals are Maxwellian averages of the following quantities:

$$\alpha = \frac{\sigma_c}{\sigma_f}$$

$$\eta = \frac{\nu\sigma_f}{\sigma_f + \sigma_c}$$

$$K_1 = (\nu - 1)\sigma_f - \sigma_c$$

The quantity K1 is known to be an especially good indicator for k_{eff}. The following is an example for U-235 from Release 3 of ENDF/B-VI:

```
thermal quantities at 300.0 K = 0.0259 eV
------------------------------------------
     fission xsec at 0.0253:  5.8472E+02
    fission nubar at 0.0253:  2.4338E+00
     capture xsec at 0.0253:  9.8575E+01
        fission xsec at tev:  5.7830E+02
       fission nubar at tev:  2.4338E+00
        capture xsec at tev:  9.7349E+01
   thermal capture integral:  8.5429E+01
   thermal capture g-factor:  9.9022E-01
capture resonance integral:  1.4337E+02
   thermal fission integral:  4.9323E+02
   thermal fission g-factor:  9.6239E-01
     thermal alpha integral:  1.6117E-01
       thermal eta integral:  2.0059E+00
        thermal k1 integral:  6.2301E+02
fission resonance integral:  2.7750E+02
------------------------------------------
```

A good reference for exerimental values of these quantities is S. F. Mughabghab, *Neutron Cross Sections, Volume I, Neutron Resonance Parameters and Thermal Cross Sections, Part B, Z=61-100,* Academic Press, 1984. Its values for the quantities in the table above are

- thermal capture cross section = 98.3 +/- 0.8 b
- thermal fission cross section = 582.6 +/- 1.1 b
- thermal nu-bar = 2.4251 +/- .0034
- thermal alpha = 0.1687 +/- .0015
- tehrmal eta = 2.0751 +/- .0033
- fission g factor = 0.9761 +/- .0012
- capture resonance integral = 144 +/- 6 b
- fission resonance integral = 275 +/- 5 b

which compare fairly well with the numbers from BROADR.

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Unresolved Resonance Self Shielding

At higher energies in heavier nuclei, the resonances get so close together that they cannot be given separately. Instead of giving individual resonances with their energies and characteristic widths, ENDF-format evaluations give average values for the resonance spacing and the various characteristic widths, together with the probability distributions needed to describe the quantities.

In this unresolved range, it is no longer possible to compute simple cross section *vs* energy tables; instead, you can calculate the effective cross section in the region of a given energy, which depends on the environment through self-shielding effects, or you can calculate probability distributions for the total cross section and the related elastic, fission, and capture distributions. The self-shielded cross sections are computed by UNRESR, and the probability tables are computed by PURR.

The effective self-shielded cross sections from UNRESR are normally used by the GROUPR module for generating self-shielded multigroup constants. The probability tables from PURR are usually processed by the ACER module and made available to the MCNP Monte Carlo code.

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Physics Add Ons To PENDF Tapes

There are a number of physical quantities that can be computed from ENDF data, but that are not explicitly included in most ENDF files. NJOY uses its data-flow model to generate such quantities and add them to a PENDF tape. Several of these physical quantities will be discussed in the following pages:

- Gas-production cross sections (sometimes called charged-particle production) are produced by the GASPR module and add to File 3 of a PENDF tape using the MT numbers from 203 (H-1 production) to 207 (He-4 production). These cross sections are normally sums over several of the reactions found on a normal ENDF-format evaluation.

- Heating and radiation damage cross sections are generated by the HEATR module and added to File 3 of a PENDF tape using special MT numbers. Values of 300+MT are used to represent heating associated with MT; normally only MT=301 for total heating is given. A special value of MT=444 is used for total radiation damage energy production, and some other values nearby are used for the components of damage, if desired.

- Thermal scattering cross sections that take the binding of the target atom into account are produced in the THERMR module. Results are added to both File 3 (cross sections) and File 6 (energy-angle distributions) using a special set of MT numbers including MT=221 for free gas scattering, MT=222 for hydrogen bound in water, and higher MT values for other important moderating materials.

The modular nature of the NJOY data-flow model allows you to include these additional physical quantities or omit them, depending on the needs of your particular applications.

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GASPR:
Gas Production Cross Sections

In many practical applications, it is important to know the total production of protons (hydrogen), alphas (helium), and other light charged particles resulting from the neutron flux. Therefore, it is convenient to have a set of special "gas production" or "charged-particle production" cross sections that can be used in application codes. The ENDF format provides a set of MT numbers for these quantities, but only a few evaluators have added them to their files:

- MT=203 -- total proton production
- MT=204 -- total deuteron production
- MT=205 -- total triton production
- MT=206 -- total He-3 production
- MT=207 -- total alpha production

The GASPR module goes through all of the reactions given in an ENDF-format evaluation, determines which charged particles would be produced by the reaction, and adds up the particle yield times the reaction cross section to produce the desired gas production cross sections. It uses data from an input ENDF tape and an input PENDF tape, and it writes the results on an output PENDF tape. They are then available for plotting, multigroup averaging, or reformatting for the MCNP Monte Carlo code.

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Gas Producing Reactions

Nuclear reactions can result in a number of different products, including photons, neutrons, light charged particles, and heavy residual nuclei. The identities of the products are sometimes implicit in the MT number for the reaction, and they are sometimes given explicitly in the section of File 6 corresponding to the reaction. When the products are implicit, they are produced with integer yields. The following table gives some common examples:

MT	products
22	1 neutron, 1 alpha, residual
103	1 proton, residual
111	2 protons, residual
113	1 triton, 2 alphas, residual

Of course, the residual could also be a light charged particle, and it may contribute to the gas production cross section.

Many of the newer evaluations now available use File 6 to provide a complete accounting of all the particles produced in a nuclear reaction, including their yields and their distributions in angle and energy. If the section in File 6 uses a simple MT number, like those tabulated above, the explicit yields will be the same as the implicit ones. However, it is also possible to use MT=5 with File 6. This MT is the sum over a number of reaction channels, and the particle yields do not have to be integers. GASPR is able to take account of these non-integer particle yields and add the correct contributions to the total gas production.

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HEATR:
Heating and Radiation Damage

Nuclear heating results from the slowing down of energetic charged particles produced in nuclear reactions, including the recoil nucleus from scattering reactions. It is a very important quantity. Sometimes it is the product being sold (as in power reactors), and sometimes it is a damaging corollary of the nuclear reactions (as in melting of important structural elements). The HEATR module of NJOY can be used to compute estimates of energy-deposition cross sections for neutrons that can be combined with calculations of neutron fluxes in nuclear systems to compute the neutronic contributions to nuclear heating. The heating due to the photon flux in a nuclear system is usually even more important; it is computed in the GAMINR module.

The same energetic charged particles and recoil nuclei that lead to heating can also cause damage to the crystalline structure of the materials that they pass through. An important case of this is the embrittlement of power reactor containment vessels that is one of the main limiting factors in the useful life of a commercial reactor. HEATR computes the damage-production energy, which can be correlated to macroscopic damage, such as tensile strength, ductility, or resistivity, through phenomenological factors like DPA (displacements per atom).

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THERMR:
Thermal Cross Sections and Scattering

At thermal energies, *e.g.*, up to about 0.5 eV for temperatures around room temperature and maybe up to as high as 4 eV for hotter materials, the energy transferred by the scattering of a neutron is similar to the kinetic energies of motion of the atoms in liquids and to the energies of excitations in molecules and crystalline lattices. Therefore, you cannot picture the target atoms as being initially stationary and recoiling freely as is normally done for higher neutron energies. The motion of the target atoms and their binding in liquids and solids affects both cross sections and the distribution in energy and angle of the scattered neutrons. The THERMR module of NJOY is used to compute these effects and add them to a PENDF tape for use by other modules.

For free-gas scattering, where only the thermal motion of the targets is taken into account, not internal modes of excitation, THERMR can generate the cross sections and scattering distributions using analytic formulas. For real bound scattering, it uses an input scattering function and other parameters from an ENDF-format thermal evaluation in File 7 format. A number of such evaluations for common moderator materials have been available for years in various ENDF-format libraries, and new ones have been produced recently using the LEAPR module of NJOY. The results of THERMR's work are stored into the new PENDF tape in Files 3 and 6 using a special set of MT numbers:

MT	Moderator
221	free gas
222	H in H_2O
223,224	H in polyethylene
225,226	H in ZrH_n
227	benzine
228	D in D_2O
229,230	C in graphite
231,232	Be
233,234	BeO
235,236	Zr in ZrH_n

As will be discussed below, the lines with two MT values refer to the inelastic and elastic components of scattering, respectively.

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THERMR: Incoherent Inelastic Scattering

The most interesting component of thermal scattering is called "incoherent inelastic" because the neutron exchanges energy with the target molecule or crystalline lattice and all the scattered waves are assumed to combine incoherently without interference effects. This component is described in terms of a scattering function called "S of alpha and beta," where alpha and beta are reduced values for momentum transfer and energy transfer, respectively:

$$\sigma^{\text{inc}}(E,E',\mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\,e^{-\beta/2}S(\alpha,\beta) ,$$

$$\beta = \frac{E'-E}{kT} ,$$

$$\alpha = \frac{E'+E-2\mu\sqrt{EE'}}{AkT} ,$$

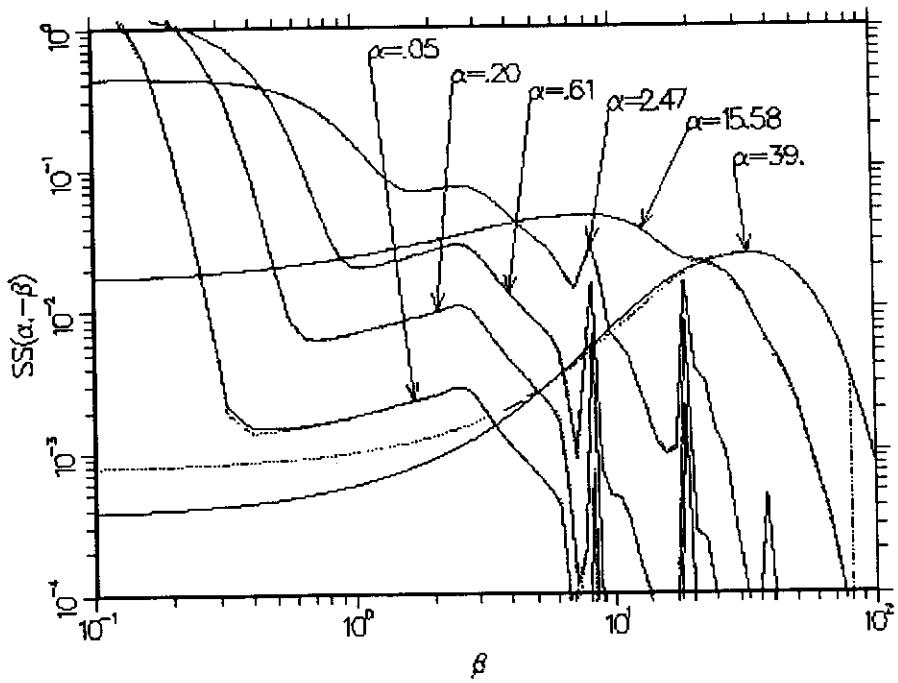
$$\sigma_b = \sigma_f\frac{(A+1)^2}{A^2} .$$

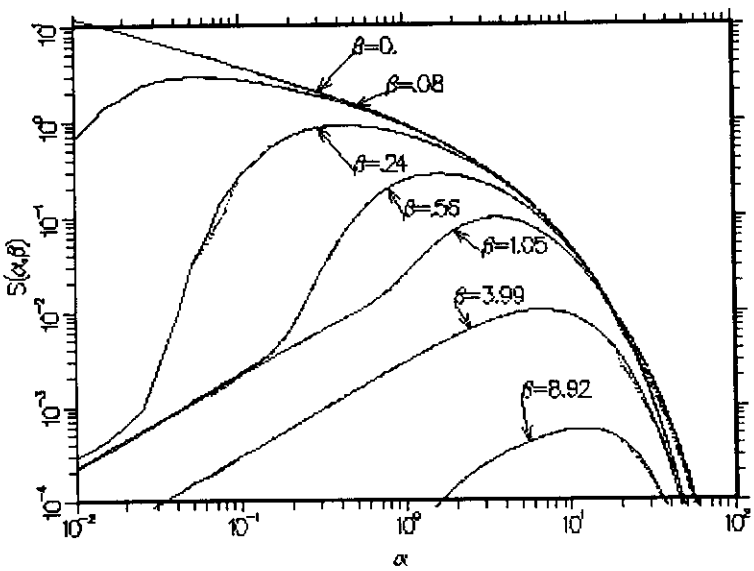
Here σ_b is the bound scattering cross section, σ_f is the free scattering cross section, E and E' are initial and final neutron energies, μ is the scattering cosine, and A is the ratio of the target mass to the neutron mass.

The scattering function for a gas of particles with no internal structure (free gas) is given by

$$S(\alpha,\beta) = \frac{1}{\sqrt{4\pi\alpha}}\exp\left\{-\frac{\alpha^2+\beta^2}{4\alpha}\right\} .$$

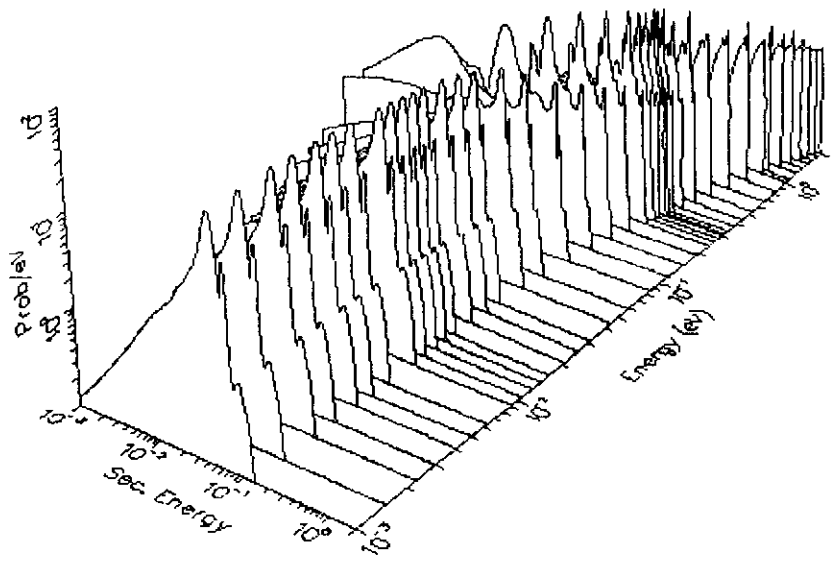
A bound scattering function is considerably more complex, as shown by the following two figures for hydrogen bound in water:





The sharp features in the first figure are due to the discrete molecular vibrations at .205 and .408 eV. The peak that develops at small alpha and beta is a pseudo-elastic peak resulting from diffusion. For more information on the physics going on in these figures, see the LEAPR write up.

THERMR processes the scattering function into an incoherent-inelastic cross section *vs* energy and a normalized energy-angle distribution. An example of such a distribution is shown below for beryllium. A number of "up-scatter" peaks corresponding to the deexitation of lattice vibrations are seen for low incident energies.



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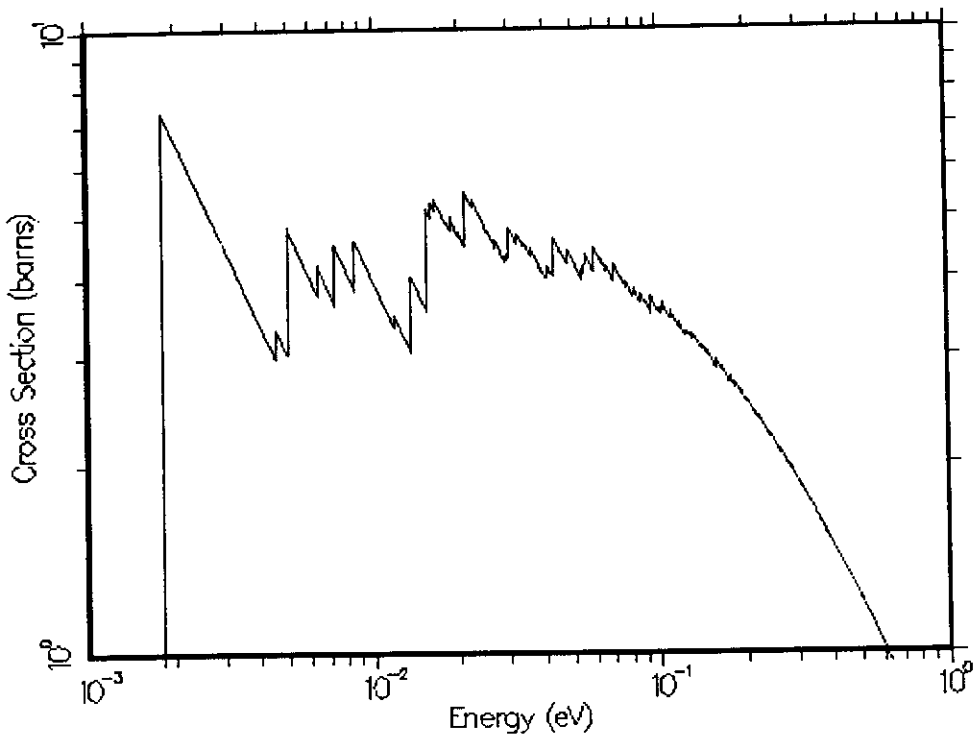
THERMR: Coherent Elastic Scattering

In crystalline materials consisting of coherent scatterers (*e.g.*, graphite, beryllium, beryllium oxide), the scattering from different planes of atoms can interfere, leading to a series of "Bragg edges" as the neutron wavelength hits various possible atomic spacings. The thermal elastic cross section of graphite is shown below:



The mathematical express of the energy-angle distribution and integrated cross section for coherent elastic scattering is as follows:

$$\sigma^{\text{coh}}(E,E',\mu) = \frac{\sigma_c}{E}\sum_{E_i<E} f_i e^{-2WE_i}\,\delta(\mu-\mu_0)\,\delta(E-E')\,,$$

$$\mu_0 = 1 - \frac{E_i}{E}\,,$$

$$\sigma^{\text{coh}} = \frac{\sigma_c}{E}\sum_{E_i>E} f_i e^{-2WE_i}\,.$$

Note that the scattering distribution is completely defined by the the energy locations and sizes of the steps in the integrated cross section. The GROUPR module and the MCNP Monte Carlo code take advantage of this feature.

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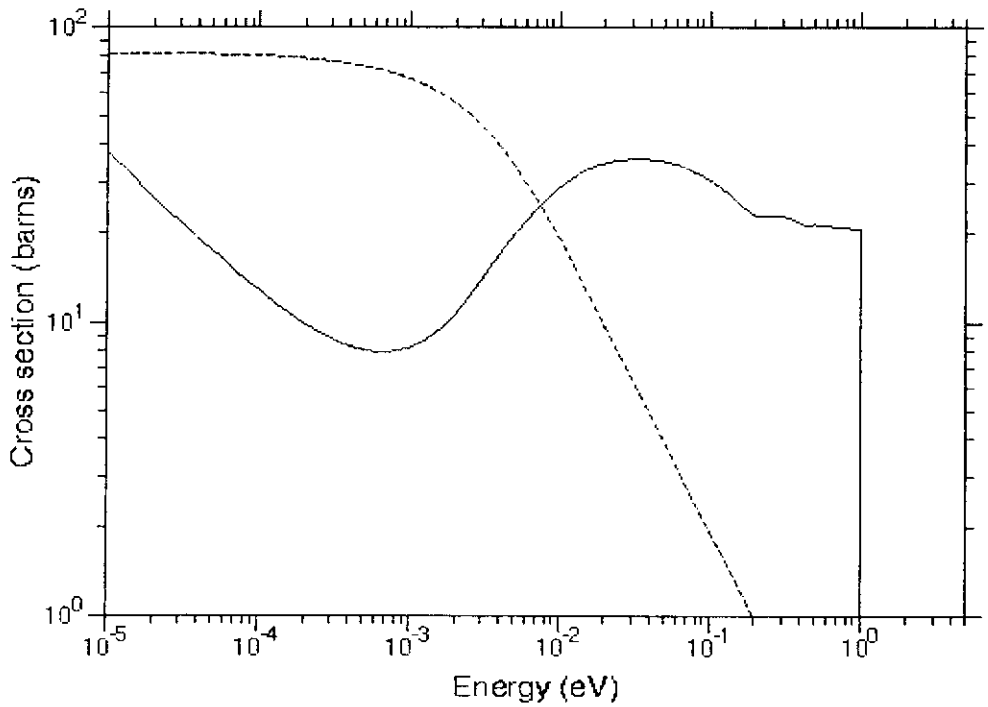
THERMR: Incoherent Elastic Scattering

In solids containing hydrogen, such as polyethylene or frozen methane, the strong incoherence of the scattering from hydrogen simplifies the elastic term:

$$\sigma^{iel}(E,E',\mu) = \frac{\sigma_b}{2} e^{-2WE(1-\mu)} \delta(E-E') ,$$

$$\sigma^{iel}(E) = \frac{\sigma_b}{2} \left\{ \frac{1-e^{-4WE}}{2WE} \right\} .$$

The cross section only depends on the bound scattering cross section and the Debye-Waller coefficient, *W*, which is computed from the excitation spectrum for the solid. The following shows an example of the elastic (dashed) and inelastic (solid) terms for frozen methane at 20K:



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THERMR:
Data Representation

The cross sections *vs* energy generated by THERMR are put into File 3 as simple tabulations using the MT number (or numbers) requested by the user. The energy-angle distributions appear as normalized distributions in File 6. For a specified grid of incident energies, a distribution *vs* secondary energy is given on a grid chosen to represent the actual angle-integrated function to a specified accuracy. At each secondary energy, a specified number of discrete scattering cosines is given with a predetermined set of probability values. This format allows for easy sampling in a Monte Carlo code, and it can also produce good values for Legendre coefficients when needed.

As an example of the THERMR run, consider the following input deck:

```
26 22 23
1065 1306 8 1 4 1 1 229 0
300.
.01 1.2
```

To understand this input, compare it with the THERMR input instructions. This run is for carbon from ENDF/B-V (MAT=1306). Thermal MAT=1065 is graphite from the thermal ENDF file Tape 322 mounted on unit 26. The results will be written on the new PENDF tape on unit 23 using MT=229 and 230.

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GROUPR: Multigroup Constants

It is very time consuming to carry out full calculations of neutron transport using the detailed PENDF cross sections that we have discussed in the preceding pages, although it can be done using continuous-energy Monte Carlo codes like MCNP, which we will discuss later. Therefore, it is very common to reduce the detail in the cross sections by averaging them over a set of energy ranges called "groups." The GROUPR module of the NJOY system carries out such averages for the pointwise cross sections, and it also generates multigroup "matrices," which describe the transfer of neutrons from one group to another.

The basis for GROUPR is the "multigroup Boltzmann transport equation," which can be written as

$$\begin{aligned} \mu\frac{\partial}{\partial x}\phi_g(x,\mu) \;+\; & \sum_{\ell=0}^{\infty} P_\ell(\mu)\sigma_{t\ell g}(x)\phi_{\ell g}(x) \\ = \; & \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\sum_{g'}\sigma_{x\ell g'\to g}(x)\phi_{\ell g'}(x) \\ + \; & Q_g(x,\mu)\,, \end{aligned}$$

where slab geometry has been used for simplicity. The first term describes the spatial transport of neutrons in group g, the second accounts for reactions in group g, the third gives the source into group g from other groups, and the last includes any fixed sources and the source from fission. The flux and cross sections that appear here are defined as follows:

$$\phi_{\ell g}(x) = \int_g \phi_\ell(x,E)\,dE\,,$$

$$\sigma_{t\ell g}(x) = \frac{\int_g \sigma_t(x,E)\phi_\ell(x,E)\,dE}{\int_g \phi_\ell(x,E)\,dE}\,.$$

$$\sigma_{x\ell g'\to g} = \frac{\int_g dE\int_{g'} dE'\,\sigma_{x\ell}(x,E'\to E)\phi_\ell(x,E')}{\int_g \phi_\ell(x,E)\,dE}\,.$$

One of the reasons for doing a transport calculation is to obtain various "responses," such heating, production of a radionuclide, or production of helium. The responses can be computed using the multigroup flux together with a multigroup reaction cross section:

$$\sigma_{rg}(x) = \frac{\int_g \sigma_r(x,E)\phi_0(x,E)\,dE}{\int_g \phi_0(x,E)\,dE}\,.$$

It is the mission of GROUPR to compute the cross sections with "g" subscripts, which are often called "multigroup constants." The Boltzmann equation itself is then solved in a separate neutron transport code, such as ANISN or DANT.

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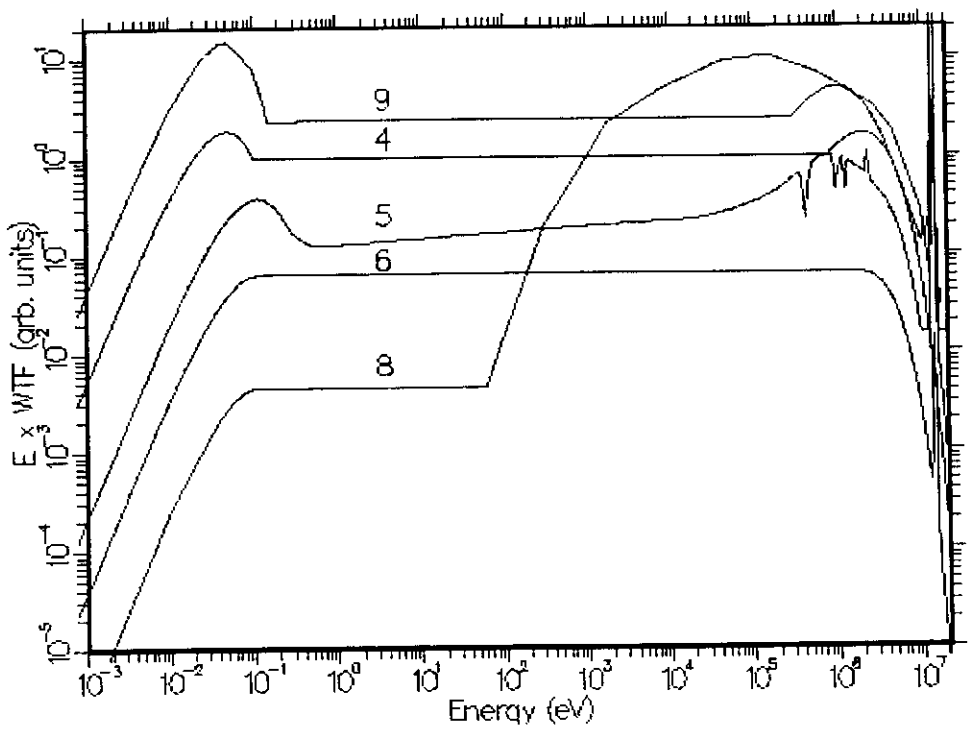
23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

GROUPR: Weighting Function

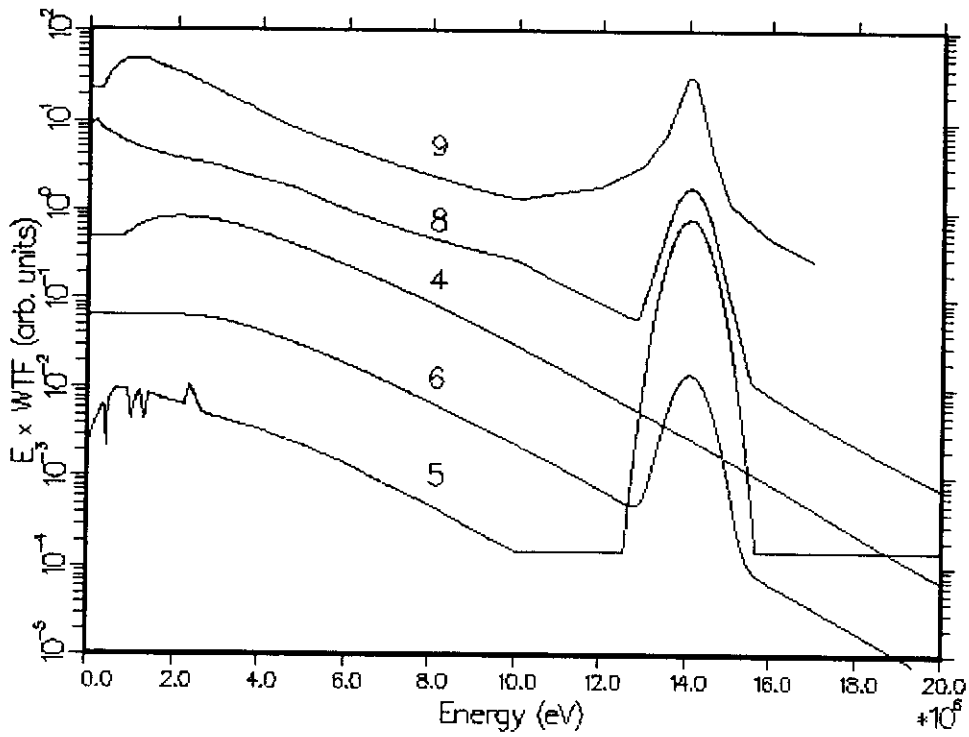
"Wait a minute," you ask, "the purpose of solving the transport equation is to get the flux, but I have to know the flux to compute the multigroup constants!" This conundrum is the source of much of the "art" in using multigroup methods. If you can make a good guess for the shape of the flux (mostly the *intragroup* flux) for the class of problems of interest, you can do very good multigroup calculations with only a few groups. If the flux can change shape between different problems or between different regions of one problem, then you have to use a large number of groups together with some default shape (such as flat weighting). The presence of resonance absorbers in a problem results in complex shapes for the weighting function, which leads to the effects called "self shielding."

As a first example, consider a typical water-moderated critical assembly, such as a power reactor. Neutrons are born at high energies (about 2 MeV) with a characteristic fission spectrum, many of them slow down by collisions with hydrogen nuclei in the water, resulting in a *1/E* shape, and they finally come into equilibrium when they reach thermal energies, resulting in a Maxwellian shape appropriate to the temperature of the system. As shown in the following figure, GROUPR contains several builtin weighting functions that show this combination of shapes:



The curves are plotted as log-log "weight per unit lethargy" or *E*W(E)*, which makes the central *1/E* part of the curve flat. The parameters used to generate the curve for IWT=4 were a thermal temperature of .0253 eV joined to *1/E* at 0.1 eV, and a fission temperature of 1.40 MeV joined to *1/E* at 820.3 keV. Curve #8 is for a fast reactor or fusion blanket.

As a second example, consider a fusion system. The neutrons born in d-T reactions appear as a sharp peak centered near 14 MeV. They then scatter down to lower energies by elastic and inelastic processes, producing a shape in the 1 MeV range very similar to the fission spectrum. If there are few light isotopes around, few neutrons get to thermal energies, and a shape like #8 results. The high-energy shapes of some of GROUPR's built-in weighting functions are shown below:



Here is a brief summary of the built-in weighting functions:

- IWT=2, constant. Used for very fine group structures like the 640-group dosimetry structure.
- IWT=3, $1/E$. Used for calculating resonance integrals.
- IWT=4, analytic thermal + $1/E$ + fission. Allows the user to adjust the relative amounts of thermal and fission flux.
- IWT=5, mid-life PWR flux spectrum with a fusion peak added. Includes some peaks and dips from oxygen, and some hardening of the $1/E$ shape. Used for EPRI data and for the LANL libraries using the WIMS structure.
- IWT=6, similar to 4, but the breakpoints were chosen to make the curve continuous and a fusion peak was added.
- IWT=7, reserved.
- IWT=8, fast reactor weighting function. It has a fusion peak and an intermediate shape typical of a fast reactor or fusion blanket. A thermal part is provided at low energies for outer regions of systems.
- IWT=9, CLAW weighting function. A typical thermal + $1/E$ + fission + fusion shape used for many years at Los Alamos.

- IWT=10, same at IWT=9, except the thermal part is automatically recalculated to follow a Maxwellian law for the actual temperature.
- IWT=11, VITAMIN-E weighting function. Another thermal + $1/E$ + fission + fusion shape.

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GROUPR: Group Structures

If the weighting function is very well known, you can do good transport calculations with very few groups, but with modern computers, the trend has been to use more and more groups. GROUPR contains a number of builtin options for group structures (some of them of mostly historical interest), and the user can enter any arbitrary structure that matches his or her needs.

Reactor physicists have always been fond the the variable called "lethargy," with is defined as follows:

$$u = \log\left(\frac{10\text{MeV}}{E}\right)$$

$$E = (10\text{MeV})e^{-u}$$

Lethargy increases as neutrons slow down. Note that in the slowing-down region, where the flux varies like *1/E*, groups with constant lethargy width all contain the same portion of the flux. In elastic scattering, neutrons loose a fraction of their energy with each scattering; thus, the lethargy increases by a fixed amount with each scattering. Because lethargy is such a natural variable for neutron slowing-down problems, many group structures are based on groups with certain lethargy widths. For example,

- the LANL 30-group structure uses "one lethargy" widths in the resonance range,
- the ANL 27-group structure uses even half-lethargy steps, and
- the GAM-I 68-group structure uses even quarter-lethargy steps.

Some group structures start with even lethargy groups and then subdivide some groups that contain especially interesting structure, such as the Fe-56 resonance at 27 keV. In other cases, the group structure starts with even lethargy groups and then moves some bounds to try to center important resonances (*e.g.*, the WIMS 69-group structure).

Another factor when choosing a group structure is its range. Many group structures intended for reactor analysis stop at 10 MeV. They are clearly not suitable for fusion problems. Other group structures only provide a few groups in the thermal range, and they are most suitable for fast-reactor and fusion problems.

The neutron group structures currently available in GROUPR are as follows:

- IGN=2, CSEWG 240-group structure, a "supergroup" structure containing bounds from many other structures. Not widely used these days.

- IGN=3, LANL 30-group structure, used for fusion problems. Still in active use.

- IGN=4, ANL 27-group structure, even half-lethargy groups used for fast-reactor analysis after collapse from more detailed structures.
- IGN=5, RRD 50-group structure, a standard fast-reactor set that is now obsolete.
- IGN=6, GAM-I 68-group structure, even quarter-lethargy set used for the epithermal part of thermal reactor codes (most recently, EPRI-CELL).
- IGN=7, GAM-II 100-group structure, an extension to higher energies of GAM-I. Note widely used these days.
- IGN=8, LASER-THERMOS 35-group structure, a thermal structure for the low energy part of power-reactor codes (most recently EPRI-CELL).
- IGN=9, EPRI-CPM 69-group structure, the WIMS structure, still widely used all over the world for reactor calculations.
- IGN=10, LANL 187-group structure, a single set of fine-lethargy bounds suitable for thermal reactors, fast reactors, and fusion reactors.
- IGN=11, LANL 70-group structure, another standard fast-reactor set, now supplanted by the 80-group structure.
- IGN=12, SAND-II 620-group structure, very fine group structure used for flux unfolding applications. Mostly supplanted by the 640-group structure.
- IGN=13, LANL 80-group structure, optimized for fast-reactor and fusion systems. Still in use through MATXS files.
- IGN=14, EURLIB 100-group structure, similar to GAM-I except for additional high-energy groups and groups near the iron resonance. Used for a number of NEA exercises.
- IGN=15, SAND-II 640-group structure, used for dosimetry work with flux unfolding codes. It extends the 620-group structure to higher energies.
- IGN=16, VITAMIN-E 174-group structure, used for the widely distributed fine-group library from Oak Ridge.
- IGN=17, VITAMIN-J 175-group structure, an extension of the 174-group structure. This structure is currently widely used in the fusion community, *e.g.*, ITER design.

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GROUPR:
Self Shielding

When the neutrons slow down in a medium with resonance absorption present, the smooth weighting function discussed above will be modified. Dips will appear in the flux corresponding to resonance peaks, and sometimes sharp peaks will occur in the flux corresponding to deep minima in the cross section, or "windows." The products of cross section and flux that appear in the definitions of the multigroup constants will clearly be reduced (self shielded) when the dips are large.

The classical method for handling self shielding in multigroup codes is the Bondarenko model. For narrow resonances in large systems, the flux takes the form:

$$\phi(E) = \frac{W(E)}{\Sigma_t(E)}$$

The denominator contains the total macroscopic cross section for the material. To obtain the part of the flux that provides self shielding for isotope *i*, it is assumed that all the other isotopes can be represented with a constant "background cross section" called σ_0. Therefore,

$$\phi^i(E) = \frac{C(E)}{\sigma_t^i(E) + \sigma_0^i}$$

The qualitative behavior of this equation is easy to understand. If σ_0 is larger than the tallest peaked in σ_t, the weighting flux is approximately proportional to the smooth weighting function *C(E)*. This is called infinite dilution; the cross section in the material of interest has little or no effect on the flux. On the other hand, if σ_0 is small with respect to σ_t, the weighting flux will have large dips at the locations of the peaks in σ_t, and a large self-shielding effect will be expected,

The following input deck will prepare self shielded cross sections for three temperatures and seven values of σ_0 for Pu-238 from ENDF/B-VI. To understand the deck, compare it with the GROUPR input instructions. A convenient way to do this is to bring the instructions up in a separate window using the right mouse button.

```
groupr
21 22 0 23
9434 6 0 4 0 3 7 1
'94-pu-238'/
300. 900. 2100.
1.e10 1.e5 1.e4 1000. 100. 10. 1
.1 0.025 0.8208e06 1.4e06
3 1 'total'/
3 2 'elastic'/
3 18 'fission'/
3 102 'capture'/
```

```
0/
3 1 'total'/
3 2 'elastic'/
3 18 'fission'/
3 102 'capture'/
0/
3 1 'total'/
3 2 'elastic'/
3 18 'fission'/
3 102 'capture'/
0/
0/
```

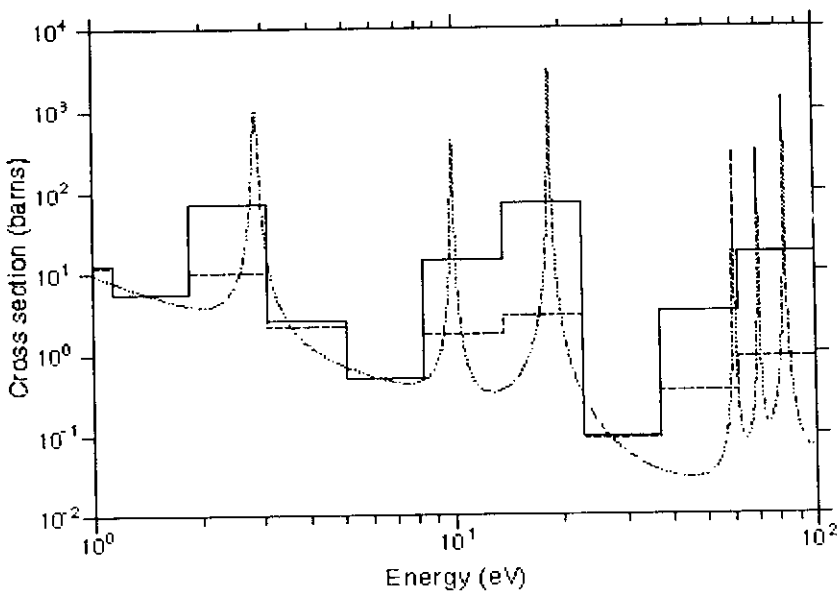
The output from GROUPR is shown below (with some excisions to make it fit the page).

```
group constants at t=3.000E+02 deg k
for mf  3 and mt102 capture

enrgy  group constants vs sigma zero
group  infinity  ... 1.000E+03  1.000E+02  1.000E+01  1.000E+00

  1    3.494E+02 ... 2.927E+02  1.995E+02  1.487E+02  1.396E+02
  2    1.254E+01 ... 1.253E+01  1.246E+01  1.227E+01  1.219E+01
  3    5.580E+00 ... 5.578E+00  5.565E+00  5.521E+00  5.495E+00
  4    7.307E+01 ... 5.052E+01  2.244E+01  1.204E+01  1.029E+01
  5    2.510E+00 ... 2.500E+00  2.434E+00  2.227E+00  2.115E+00
  6    5.200E-01 ... 5.200E-01  5.198E-01  5.189E-01  5.181E-01
  7    1.425E+01 ... 1.099E+01  4.944E+00  2.225E+00  1.743E+00
  8    7.344E+01 ... 2.738E+01  8.348E+00  3.696E+00  2.899E+00
  9    9.300E-02 ... 9.297E-02  9.275E-02  9.174E-02  9.083E-02
 10    3.183E+00 ... 2.645E+00  1.262E+00  4.791E-01  3.409E-01
 11    1.694E+01 ... 8.739E+00  2.943E+00  1.165E+00  8.858E-01
 12    2.627E+01 ... 1.489E+01  5.083E+00  1.979E+00  1.488E+00
 13    2.337E+01 ... 1.254E+01  4.472E+00  1.981E+00  1.592E+00
 14    1.348E+01 ... 8.083E+00  3.312E+00  1.459E+00  1.123E+00
 15    1.081E+01 ... 6.994E+00  3.060E+00  1.373E+00  1.056E+00
 16    7.869E+00 ... 5.761E+00  2.772E+00  1.277E+00  9.828E-01
 17    6.324E+00 ... 4.939E+00  2.560E+00  1.219E+00  9.415E-01
 18    5.154E+00 ... 4.223E+00  2.352E+00  1.165E+00  9.056E-01
 19    4.195E+00 ... 3.579E+00  2.141E+00  1.109E+00  8.704E-01
```

And finally, we show a plot of the PENDF cross section for capture (dotted), the infinitely-dilute capture (solid), and the self-shielded capture for a background cross section of 1 barn (dashed).



GROUPR:
Multigroup Matrices

In order to unify several different processing tasks, GROUPR uses the concept of a generalized group integral

$$\sigma_g = \frac{\int_g \mathcal{F}(E)\,\sigma(E)\,\phi(E)\,dE}{\int_g \phi(E)\,dE},$$

where the integrals are over all initial neutron energies in group g, $\sigma(E)$ is a cross section at E, and $\phi(E)$ is an estimate of the flux at E. We call fancy F of $E$the "feed function". It alone changes for different data types. To average a neutron cross section, fancy F is set to 1. To average a ratio quantity like fission mubar with respect to elastic scattering, fancy F is set to mu. For photon production, fancy F is the photon yield. For matrices, it is the l-th Legendre component of the normalized probability of scattering into secondary energy group g' from initial energy E. This definition is clearly independent of whether the secondary particle is a neutron or a photon.

The question of integration grid or quadrature scheme is important for the evaluation this equation. Each factor in the integrands has its own characteristic features, and it is important to account for them all. First, a grid must be established for each factor. As an example, the grid of $\sigma(E)$ is generated in RECONR and BROADR such that sigma can be obtained to within a given tolerance by linear interpolation. GROUPR contains a subroutine GETSIG which carries out this interpolation at E and also returns the next grid energy in ENEXT. Subroutines GETFLX and GETFF perform similar functions for the flux and feed function. It is now easy to generate a union grid for the three-factor integrand by just selecting the next closest ENEXT from all the factors at each step of the integration.

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GROUPR:
Two-Body Scattering

Elastic scattering (ENDF MT=2) and discrete inelastic neutron scattering (with MT=51-90) are both examples of two-body kinematics and are treated together by GROUPR. The feed function required for the group-to-group matrix calculation may be written

$$\mathcal{F}_{\ell g'}(E) = \int_{g'} dE' \int_{-1}^{+1} d\omega \, f(E \to E', \omega) \, P_\ell(\mu[\omega]) \, ,$$

where $f(E,E',\omega)$ is the probability of scattering from E to E' through a center-of-mass cosine ω and P_{ls} is a Legendre polynomial for laboratory cosine μ. The laboratory cosine corresponding to ω is given by

$$\mu = \frac{1 + R\omega}{\sqrt{1 + R^2 + 2R\omega}} \, ,$$

and the cosine ω is related to secondary energy E' by

$$\omega = \frac{E'(1+A)^2/A' - E(1+R^2)}{2RE} \, ,$$

where A' is the ratio of the emitted particle mass to the incident particle mass (A'=1 for neutron scattering). In these equations, R is the effective mass ratio

$$R = \sqrt{\frac{A(A+1-A')}{A'}} \sqrt{1 - \frac{(A+1)(-Q)}{AE}} \, ,$$

where A is the ratio of target mass to neutron mass, and $-Q$ is the energy level of the excited nucleus (Q=0 for elastic scattering). Integrating the defining equation for the two-body feed function over secondary energy gives

$$\mathcal{F}_{\ell g'}(E) = \int_{\omega_1}^{\omega_2} f(E, \omega) \, P_\ell(\mu[\omega]) \, d\omega \, ,$$

where ω_1 and ω_2 are evaluated using the kinematics equations with E' equal to the upper and lower bounds of g', respectively. The scattering probability is given by

$$f(E, \omega) = \sum_{\ell=0}^{L} f_\ell(E) \, P_\ell(\omega) \, ,$$

where the Legendre coefficients are either retrieved directly from the ENDF/B

File 4 or computed from File 4 tabulated angular distributions using subroutines from the GROUPR module called GETFLE and GETCO.

The integration over ω is performed simultaneously for all Legendre components using Gaussian quadrature. The quadrature order is selected based on an estimate of the polynomial order of the integrand using the known order of the CM angular distribution plus a factor depending on atomic weight ratio AWR. More terms are needed for light targets.

The resulting two-body feed function for higher Legendre orders is a strongly oscillatory function of incident energy in some energy ranges. Such functions are very difficult to integrate with adaptive techniques. Gaussian methods, on the other hand, are capable of integrating such oscillatory functions exactly if they are polynomials. Since a polynomial representation of the feed function is fairly accurate, a Gaussian quadrature scheme was chosen for GROUPR. The scheme used is also well adapted to performing many integrals in parallel. In GROUPR, all Legendre components and all final groups are accumulated simultaneously. NJOY takes pains to locate the "critical points" in incident energy so that the Gaussian integrations are performed over energy ranges that do not contain discontinuities. Here is an example of a multigroup elastic scattering matrix for carbon computed using GROUPR for a 30-group structure:

```
group constants at t=3.000E+02 deg k                                    16.
for mf  6 and mt  2 elastic

initl  final  group constants vs legendre order
group  group  0          1          2          3

  1      1    8.087E+00  4.532E-01  1.144E-02  4.205E-05
  2      1    7.572E-01 -2.232E-01 -1.690E-02 -4.363E-04
  2      2    4.003E+00  4.900E-01  2.363E-02  4.544E-04
  3      2    7.525E-01 -2.219E-01 -1.676E-02 -4.303E-04
  3      3    3.995E+00  4.879E-01  2.348E-02  4.484E-04
  4      3    7.574E-01 -2.234E-01 -1.686E-02 -4.318E-04
  4      4    3.985E+00  4.891E-01  2.357E-02  4.498E-04
  5      4    7.539E-01 -2.223E-01 -1.678E-02 -4.294E-04
  5      5    3.986E+00  4.880E-01  2.348E-02  4.474E-04
   ...
 28     26    8.308E-02 -4.928E-02  8.439E-03  1.234E-02
 28     27    2.545E-01  7.532E-02 -6.513E-03  2.423E-02
 28     28    5.256E-01  4.740E-01  3.849E-01  2.805E-01
 29     26    4.329E-03 -4.075E-03  3.606E-03 -2.988E-03
 29     27    1.217E-01 -4.973E-02 -1.258E-02  1.592E-02
 29     28    1.841E-01  1.053E-01  2.710E-02  4.737E-04
 29     29    5.124E-01  4.633E-01  3.788E-01  2.799E-01
 30     27    2.721E-02 -2.127E-02  1.255E-02 -5.134E-03
 30     28    6.865E-02 -1.719E-02 -1.846E-02  1.032E-02
 30     29    1.834E-01  1.016E-01  1.937E-02 -7.491E-03
 30     30    6.055E-01  5.428E-01  4.372E-01  3.182E-01
```

Note that the "in-group" cross section is much larger than the outscattering cross section, which is normally limited to a fairly small energy loss by kinematics. Also note that the scattering tends to be fairly isotropic at low

energies (low group numbers here), but it becomes very forward peaked for in-scatter in group 30. This is demonstrated by the slow decrease for higher Legendre orders (a delta function of forward scattering would have the same cross section for each l order).

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GROUPR:
Continuum Scattering and Fission

In ENDF/B, scattering from many closely-spaced levels or multibody scattering such as (n,2n), (n,n'α), and fission can be represented using a separable function of scattering cosine and secondary neutron energy

$$f(E \to E', \mu) = F(E, \mu)\, g(E \to E') \ ,$$

where F is the probability that a neutron will scatter through a laboratory angle with cosine μ irrespective of final energy E'. It is obtained from MF=4. Similarly, g is the probability that a neutron's energy will change from E to E' irrespective of the scattering angle, and it is given in MF=5. Continuum reactions are easily identified by MT numbers of 6-49 and 91. The secondary-energy distributions can be represented using a two-dimensional tabulation or using an analytic law. The feed functions for continuum scattering are simply

$$\mathcal{F}_{\ell g'}(E') = \int_{-1}^{+1} P_\ell(\mu)\, f(E, \mu)\, d\mu \int_{g'} g(E, E')\, dE' \ .$$

and the cosine omega is related to secondary energy E' by

$$\mathcal{F}_{0g'}(E') = \int_{g'} g(E, E')\, dE' \ .$$

As discussed in the companion article in this volume "An Introduction to the ENDF Formats," the separability assumption is no longer considered adequate for reaction like (n,2n) or (n,n'α), because it doesn't describe the energy-angle correlation that occurs for these reactions. As a result, the continuum approach is only found for old carry-over materials and for minor actinides or fission products where neutron transport is a secondary concern. In these cases, the angular distribution is almost invariably given as isotropic in the laboratory system. However, the continuum approach remains the method of choice for fission, which is also modeled as isotropic in the laboratory frame. Therefore, in almost all cases of interest, the feed function reduces to

$$\mathcal{F}_{0g'}(E') = \int_{g'} g(E, E')\, dE' \ .$$

The integrals on the right hand side are returned by the GROUPR subroutine GETSED (for get secondary energy distribution), which either interpolates and integrates over the tabulation, or uses direct analytical integrals, as required. The integration over incident energy proceeds as for all other GROUPR

quantities. The result in a scattering or fission matrix, $\sigma_{gg'}$. For scattering, the matrix will contain only downscattering elements for groups g from the threshold up. For fission, the matrix can be almost completely full with both energy increase and energy loss elements.

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GROUPR:
Fission Source, Nubar, and Chi

As discussed above, the natural representation of fission in GROUPR is a a group-to-group transfer matrix, $\sigma_{gg'}$. But the quantity required for the multigroup Boltzmann transport equation is the fission source into group g,

$$S_g = \sum_{g'} \sigma_{fg' \to g} \phi_{0g'} ,$$

Most existing transport code packages are not able to use a full fission matrix directly to compute this fission source; instead they count on the observation that, except for relatively high neutron energies, the spectrum of fission neutrons is only weakly dependent on initial energy. Therefore, the fission source can be written

$$S_g = \chi_g \sum_{g'} \bar{\nu}_{g'} \sigma_{fg'} \phi_{0g'} ,$$

where nu_g is the fission neutron yield, σ_{fg} is the fission cross section, and χ_g is the average fission spectrum (the familiar "chi" vector), which can be defined by

$$\chi_g = \frac{\sum_{g'} \sigma_{fg' \to g} \phi_{0g'}}{\sum_{g} \sum_{g'} \sigma_{fg' \to g} \phi_{0g'}} , .$$

The fission neutron yield is given by

$$\bar{\nu}_g = \sum_{g'} \sigma_{fg \to g'} / \sigma_{fg} .$$

Clearly, χ_g computed in this way depends on the flux in the system of interest. In most cases, the built in weighting functions in GROUPR are not adequate for computing χ_g; they are really only intended to provide reasonable *intragroup* fluxes. For this reason, GROUPR does not attempt to compute the fission chi itself--it just passes on the full fission matrix to some subsequent code that allows the user to enter an appropriate flux spectrum. Because the energy dependence is weak except for high incident energies, a rough guess for ϕ_{0g} usually gives an accurate fission chi. When this is not the case, the problem can be iterated. The DTFR and WIMSR modules know how to calculate chi from GROUPR output, and the TRANSX code working with

MATXS files can support the fission-spectrum iteration described above.

There is an addition complication for fission. The fission matrix from GROUPR only describes the prompt part of fission. It is also necessary to obtain the delayed neutron yield and spectra from GROUPR and combine them with the prompt matrix to contain the complete total fission nubar and chi.

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GROUPR:
Running GROUPR

Setting up GROUPR runs can be daunting, because it has many possibilities for giving the user complete control over which reactions and data types are processed. However, for many applications, the user can use automatic modes that greatly simplify the input. Here is a simple example of a deck that computes infinitely dilute cross sections for carbon using a built-in group structure and weight function.

```
groupr
20 21 0 22 / ENDF on tape20, PENDF on tape21, GENDF on tape22
1306 3 3 3 3 1 1 1 / 30 groups, CLAW weight, P3
'carbon from ENDF/B-V'/
300 / one temperature
1.e10 / infinite dilution only
3/ process all cross sections on PENDF
6/ process all matrices
16/ process all photon production reactions
0/ end of this temperature
0/ end of groupr input
```

A clearer understanding of this input lines can be obtained by studying the GROUPR input specifications in the online version, a printed NJOY manual, or the files in the NJOY distribution. The notes after the "slash" terminator explain most of the features of this input deck.

Because not all user need all possible reactions, the automatic input process skips over thermal data (MT=221--250) and delayed neutron data (MT=455). If you need thermal data to be group averaged, include something like this in your deck:

```
3/ all reactions but thermal
3 229 'graphite inelastic'/
3 230 'graphite elastic'/
6/ all matrices but thermal
6 229 'graphite inelastic'/
6 230 'graphite elastic'/
```

Similarly, if you need delayed-neutron production and spectra, include something like this in your deck:

```
3 455/ delayed nubar
5 455/ delayed spectra
```

The code will automatically provide spectra for all the six time groups of delayed neutrons. As discussed in the previous subsection, it is the

responsibility of a subsequent code to merge the delayed neutron data with the prompt data for the calculation of a proper fission source. As a final example, to obtain self-shielded cross sections and scattering matrices, you have to ask for several temperatures and several σ_0 values. It is not necessary to reprocess all the reactions at the higher temperatures; just include the reactions that occur at resonance energies:

```
groupr
20 21 0 22
1050 3 0 3 3 2 3 1
'94-pu-238 from ENDF/B-IV'/
300 900
1e10 1e4 1000 100 10 1
3/ all reactions at 300K
6/ all matrices at 300K
0/ end of first temperature (300K)
3 1 'total'/ only resonance reactions at 900K
3 2 'elastic'/
3 18 'fission'/
3 102 'capture'/
6 2 'elastic'/ yes, you can self shield the elastic matrix
0/ end of second temperature (900K)
0/ end of groupr deck
```

GROUPR has other capabilities, including custom group structures, custom weight functions, the flux calculator, charged particle transfer matrices, and activation cross section processing, that can be explored in the detailed documentation

NEXT INDEX

ACER:
Monte Carlo Libraries

In these days of inexpensive fast computers with huge memories, people are making more and more use of detailed Monte Carlo transport calculations. This approach is much more expensive than the multigroup approach, but it has two great advantages:

- detailed cross sections don't have to be approximated, and
- simplified models of the geometry don't have to be used.

There are Monte Carlo codes (*e.g.*, MORSE) that use multigroup data, and NJOY's multigroup data can be reformatted for these codes, but the most faithful physics modeling can be obtained by using a full continuous-energy Monte Carlo code like MCNP from Los Alamos. NJOY can produce libraries for the MCNP code by using its ACER module. Here is an example of how we normally do this using a unix script:

```
echo "ACE production and testing run:"
echo "getting files"
cfs get tape20:/endf/6u/neutron/c/nata    [This is an existing ENDF tape]
cfs get tape21:/pendf/6u/c/nata           [This is an existing PENDF tape]
cat input EOF
 acer
 20 21 0 31 32
     1 0 1/ fast data, no listing, type-1 format (ASCII)
 '6-c-nata from endf-vi.1'/
 600 296.3/ MAT and temperature
 .01/ thin distributions to 1%
 /
 acer
 0 31 33 34 35 / file33 is plotting output
 7 1 2/ read type-1 file, make listing, write type-2 file (binary)
 '6-c-nata from endf-vi.1'/
 viewr
 33 36/ convert the acer plot output to postscript
 stop
EOF
echo "running njoy"
xnjoy input
echo "saving njoy output"
cfs store dir=/acer/6u/f/c output:natao tape31:nata tape32:natax
cfs store dir=/acer/6u/f/c tape33:natav tape36:natap
echo "creating local xsdir file for material test ..."
cfs get /acer/xsdir2
xsdir2  EOF
/acer/6u/f/c/nata
EOF
echo "creating mcnp inp file for material test ..."
cat inp EOF
```

NEXT INDEX

---

23 January 1998 T-2 Nuclear Information Service *ryxm@lanl.gov*

Input Instructions for NJOY

```
*****************************************************************
*                                                               *
* card 1        module option                                   *
*                                                               *
*    module     six character module name, e.g., reconr.       *
*               it is not necessary to use quotes.              *
*                                                               *
*          repeat card 1 for each module desired, and           *
*          use the name "stop" to terminate program.            *
*                                                               *
*  follow the module name with the specific input               *
*  instructions for that particular module.                     *
*                                                               *
*****************************************************************
```

Input Instructions for RECONR

```
**********************************************************************
*                                                                    *
* card 1                                                             *
*    nendf     unit for endf/b tape                                  *
*    npend     unit for pendf tape                                   *
* card 2                                                             *
*    tlabel    66 character label for new pendf tape                 *
*              delimited with quotes, ended with /.                  *
* card 3                                                             *
*    mat       material to be reconstructed                          *
*    ncards    number of cards of descriptive data for new mf1       *
*              (default=0.)                                          *
*    ngrid     number of user energy grid points to be added.        *
*              (default=0.)                                          *
* card 4                                                             *
*    err       fractional reconstruction tolerance used when         *
*              resonance-integral error criterion (see errint)       *
*              is not satisfied.                                     *
*    tempr     reconstruction temperature (deg kelvin)               *
*              (default=0.)                                          *
*    errmax    fractional reconstruction tolerance used when         *
*              resonance-integral error criterion is satisfied       *
*              (errmax.ge.err, default=20.*err)                      *
*    errint    maximum resonance-integral error (in barns)           *
*              per grid point (default=err/10000)                    *
*              (note: the max cross section difference for           *
*              linearization, errlim, and for reconstruction,        *
*              errmin, are also tied to errint.  to get maximum      *
*              accuracy, set errint to a very small number.          *
*              for economical production, use the defaults.)         *
* card 5                                                             *
*    cards     ncards of descriptive comments for mt451              *
*              each card delimited with quotes, ended with /.        *
* card 6                                                             *
*    enode     users energy grid points                              *
*                                                                    *
*     cards 3, 4, 5, 6 must be input for each material desired       *
*     mat=0/ terminates execution of reconr.                         *
*                                                                    *
**********************************************************************
```

Input Instructions for BROADR

```
*****************************************************************
*                                                               *
* card 1                                                        *
*    nendf     input endf tape (for thermal nubar only)         *
*    nin       input pendf tape                                 *
*    nout      output pendf tape                                *
* card 2                                                        *
*    mat1      material to be processed                         *
*    ntemp2    number of final temperatures (maximum=10)        *
*    istart    restart (0 no, 1 yes, default 0)                 *
*    istrap    bootstrap (0 no, 1 yes, default 0)               *
*    temp1     starting temperature from nin (default=0.k)      *
* card 3                                                        *
*    errthn    fractional tolerance for thinning                *
*    thnmax    max. energy for broadening and thinning          *
*              (default=1 mev)                                  *
*    errmax    fractional tolerance used when integral criterion *
*              is satisfied (same usage as in reconr)           *
*              (errmax.ge.errthn, default=20*errthn)            *
*    errint    parameter to control integral thinning           *
*              (usage as in reconr) (default=errthn/10000)      *
*              set very small to turn off integral thinning.    *
*      (a good choice for the convergence parameters            *
*       errthn, errmax, and errint is the same set of           *
*       values used in reconr)                                  *
* card 4                                                        *
*    temp2     final temperatures (deg kelvin)                  *
* card 5                                                        *
*    mat1      next mat number to be processed with these       *
*              parameters.  terminate with mat1=0.              *
*                                                               *
*---input options-----------------------------------------------*
*                                                               *
* the output tape will contain the ntemp2 final temperatures    *
* specified.  it is necessary to have temp1.le.temp2(1).        *
* if temp2.eq.temp1, the data will be thinned only.             *
*                                                               *
* restart    continue broadening an existing pendf tape.  all   *
*            temperatures are copied through temp1.  additional *
*            final temperatures are added by starting with the  *
*            data at temp1.                                     *
*                                                               *
* bootstrap  if bootstrap is not requested, each final tempera- *
*            ture is generated by broadening directly from      *
*            temp1 to temp2.  if bootstrap is requested, each   *
*            final temperature is broadened from the preceding  *
*            temperature.  this option is faster due to the     *
*            thinning in the previous step.  however, errors    *
*            accumulate.                                        *
*                                                               *
* thnmax     the upper limit for broadening and thinning is the *
*            lowest of the input value of thnmax, the lowest    *
*            reaction threshold, or the start of the unresolved *
*            range.  if there is resolved-unresolved overlap,   *
*            the overlap region is included in the broadening.  *
*            a negative value of thnmax will override the       *
*            resolved and threshold limits.  This allows the    *
*            first few threshold reactions to be broadened if   *
*            desired.  the magnitude of thnmax must be chosen   *
*            to keep the number of broadenable reactions less   *
*            than or equal to the maximum of ntt (10).          *
*                                                               *
*****************************************************************
```

Input Instructions for UNRESR

```
*****************************************************************
*                                                               *
* card 1                                                        *
*   nendf   unit for endf/b tape                                *
*   nin     unit for input pendf tape                           *
*   nout    unit for output pendf tape                          *
* card 2                                                        *
*   matd    material to be processed                            *
*   ntemp   no. of temperatures (10 max)                        *
*   nsigz   no. of sigma zeroes (10 max)                        *
*   iprint  print option (0=min, 1=max) (default=0)              *
* card 3                                                        *
*   temp    temperatures in kelvin (including zero)             *
* card 4                                                        *
*   sigz    sigma zero values (including infinity)              *
*       cards 2, 3, 4 must be input for each material desired    *
*       matd=0/ terminates execution of unresr.                 *
*                                                               *
*****************************************************************
```

Input Instructions for HEATR

```
*********************************************************************
*                                                                   *
* card 1                                                            *
*    nendf     unit for endf/b tape                                 *
*    nin       unit for input pendf tape                            *
*    nout      unit for output pendf tape                           *
*    nplot      unit for graphical check output                     *
* card 2                                                            *
*    matd      material to be processed                             *
*    npk       number of partial kermas desired (default=0)         *
*    nqa       number of user q values (default=0)                  *
*    ntemp     number of temperatures to process                    *
*              (default=0, meaning all on pendf)                    *
*    local     0/1=gamma rays transported/deposited locally         *
*              (default=0)                                          *
*    iprint    print (0 min, 1 max, 2 check) (default=0)            *
* card 3       for npk gt 0 only                                    *
*    mtk       mt numbers for partial kermas desired                *
*              total (mt301) will be provided automatically.        *
*              partial kerma for reaction mt is mt+300              *
*              and may not be properly defined unless               *
*              a gamma file for mt is on endf tape.                 *
*              special values allowed--                             *
*                303   non-elastic (all but mt2)                    *
*                304   inelastic (mt51 thru 91)                     *
*                318   fission (mt18 or mt19, 20, 21, 38)           *
*                401   disappearance (mt102 thru 120)               *
*                443   total kinematic kerma (high limit)           *
*              damage energy production values--                    *
*                444   total                                        *
*                445   elastic (mt2)                                *
*                446   inelastic (mt51 thru 91)                     *
*                447   disappearance (mt102 thru 120)               *
*           cards 4 and 5 for nqa gt 0 only                         *
* card 4                                                            *
*    mta       mt numbers for users q values                        *
* card 5                                                            *
*    qa        user specified q values (ev)                         *
*                (if qa.ge.99.e6, read in variable qbar             *
*                   for this reaction)                              *
* card 5a      variable qbar (for reactions with qa flag only)      *
*    qbar       tab1 record giving qbar versus e (1000 words max)   *
*                                                                   *
*********************************************************************
```

Input Instructions for THERMR

```
*********************************************************************
*                                                                   *
*  card 1                                                           *
*     nendf       endf/b tape for mf7 data                          *
*     nin         old pendf tape                                    *
*     nout        new pendf tape                                    *
*  card 2                                                           *
*     matde       material desired on endf tape                     *
*     matdp       material desired on pendf tape                    *
*     nbin        number of equi-probable angles                    *
*     ntemp       number of temperatures                            *
*     iinc        inelastic options                                 *
*                    0     none                                     *
*                    1     compute as free gas                      *
*                    2     reserved                                 *
*                    3     reserved                                 *
*                    4     read s(a,b) and compute matrix           *
*     icoh        elastic options                                   *
*                    0     none                                     *
*                    1     graphite                                 *
*                    2     beryllium                                *
*                    3     beryllium oxide                          *
*                   11     polyethylene                             *
*                   12     h(zrh)                                   *
*                   13     zr(zrh)                                  *
*     natom       number of principal atoms                         *
*     mtref       mt for inelastic reaction (201-250 only)          *
*     iprint      print option (0=minimum, 1=maximum,               *
*                 2=max. normal + intermediate results)             *
*                 (default=0)                                       *
*  card 3                                                           *
*     tempr       temperatures (kelvin)                             *
*  card 4                                                           *
*     tol         tolerance                                         *
*     emax        maximum energy for thermal treatment              *
*                 (for temperatures greater than 3000,              *
*                 emax and the energy grid are scaled by            *
*                 temp/300.  free gas only.)                        *
*                                                                   *
*       nendf can be endf-6 format (e.g., from leapr) while         *
*       nin and nout are endf-4 or 5 format, if desired.            *
*                                                                   *
*********************************************************************
```

Input Instructions for GROUPR

```
*********************************************************************
*                                                                   *
* card1                                                             *
*    nendf   unit for endf/b tape                                   *
*    npend   unit for pendf tape                                    *
*    ngout1  unit for input gout tape (default=0)                   *
*    ngout2  unit for output gout tape (default=0)                  *
* card2                                                             *
*    matb    material to be processed                               *
*            matb lt 0 is a flag to add mts to and/or replace       *
*            individual mts on ngout1.                              *
*    ign     neutron group structure option                         *
*    igg     gamma group structure option                           *
*    iwt     weight function option                                 *
*    lord    legendre order                                         *
*    ntemp   number of temperatures                                 *
*    nsigz   number of sigma zeroes                                 *
*    iprint  long print option (0/1=minimum/maximum)                *
*            (default=1)                                            *
* card3                                                             *
*    title   run label (up to 80 characters delimited by *,         *
*            ended with /)  (default=blank)                         *
* card4                                                             *
*    temp    temperatures in kelvin                                 *
* card5                                                             *
*    sigz    sigma zero values (including infinity)                 *
*                                                                   *
*          if ign=1, read neutron group structure (6a and 6b)       *
* card6a                                                            *
*    ngn     number of groups                                       *
* card6b                                                            *
*    egn     ngn+1 group breaks (ev)                                *
*                                                                   *
*          if igg=1, read gamma group structure (7a and 7b)         *
* card7a                                                            *
*    ngg     number of groups                                       *
* card7b                                                            *
*    egg     ngg+1 group breaks (ev)                                *
*                                                                   *
*          weight function options (8a,8b,8c,8d)                    *
* card8a     flux calculator parameters (iwt.lt.0 only)             *
*    ehi     break between computed flux and bondarenko flux        *
*                (must be in resolved range)                        *
*    sigpot  estimate of potential scattering cross section         *
*    nflmax  maximum number of computed flux points                 *
*    ninwt   tape unit for new flux parameters (default=0)          *
*    jsigz   index of reference sigma zero in sigz array            *
*            (default=0)                                            *
*    alpha2   alpha for admixed moderator (def=o=none)              *
*    sam      admixed moderator xsec in barns per absorber          *
*             atom (def=0=none)                                     *
*    beta     heterogeniety parameter (def=0=none)                  *
*    alpha3   alpha for external moderator (def=0=none)             *
*    gamma    fraction of admixed moderator cross section in        *
*              external moderator cross section (def=0)             *
* card8b     tabulated (iwt=1 or -1 only)                           *
*    wght    read weight function as tab1 record.                   *
*            end with a /.                                          *
* card8c     analytic flux parameters (iwt=4 or -4 only)            *
*    eb      thermal break (ev)                                     *
*    tb      thermal temperature (ev)                               *
*    ec      fission break (ev)                                     *
*    tc      fission temperature (ev)                               *
* card8d     input resonance flux (iwt=0 only)                      *
*    ninwt   tape unit for flux parameters                          *
*                                                                   *
```

```
* card9                                                              *
*    mfd      file to be processed                                   *
*    mtd      section to be processed                                *
*    mtname   description of section to be processed                 *
*          repeat for all reactions desired                         *
*          mfd=0/ terminates this temperature/material.             *
* card10                                                             *
*    matd     next mat number to be processed                        *
*             matd=0/ terminates groupr run.                         *
*                                                                    *
*---options for input variables---------------------------------------*
*                                                                    *
*     ign          meaning                                         *
*     ---          -------                                         *
*      1           arbitrary structure (read in)                   *
*      2           csewg 239-group structure                       *
*      3           lanl 30-group structure                         *
*      4           anl 27-group structure                          *
*      5           rrd 50-group structure                          *
*      6           gam-i 68-group structure                        *
*      7           gam-ii 100-group structure                      *
*      8           laser-thermos 35-group structure                *
*      9           epri-cpm 69-group structure                     *
*     10           lanl 187-group structure                        *
*     11           lanl 70-group structure                         *
*     12           sand-ii 620-group structure                     *
*     13           lanl 80-group structure                         *
*     14           eurlib 100-group structure                      *
*     15           sand-iia 640-group structure                    *
*     16           vitamin-e 174-group structure                   *
*     17           vitamin-j 175-group structure                   *
*                                                                  *
*     igg          meaning                                         *
*     ---          -------                                         *
*      0           none                                            *
*      1           arbitrary structure (read in)                   *
*      2           csewg 94-group structure                        *
*      3           lanl 12-group structure                         *
*      4           steiner 21-group gamma-ray structure            *
*      5           straker 22-group structure                      *
*      6           lanl 48-group structure                         *
*      7           lanl 24-group structure                         *
*      8           vitamin-c 36-group structure                    *
*      9           vitamin-e 38-group structure                    *
*     10           vitamin-j 42-group structure                    *
*                                                                  *
*     iwt          meaning                                         *
*     ---          -------                                         *
*      1           read in smooth weight function                  *
*      2           constant                                        *
*      3           1/e                                             *
*      4           1/e + fission spectrum + thermal maxwellian     *
*      5           epri-cell lwr                                   *
*      6           (thermal) -- (1/e) -- (fission + fusion)        *
*      7           same with t-dep thermal part                    *
*      8           thermal--1/e--fast reactor--fission + fusion    *
*      9           claw weight function                            *
*     10           claw with t-dependent thermal part              *
*     11           vitamin-e weight function (ornl-5505)           *
*     12           vit-e with t-dep thermal part                   *
*     -n           compute flux with weight n                      *
*      0           read in resonance flux from ninwt               *
*                                                                  *
*     mfd          meaning                                         *
*     ---          -------                                         *
*      3           cross section or yield vector                   *
*      5           fission chi by short-cut method                 *
*      6           neutron-neutron matrix (mf4/5)                  *
*      8           neutron-neutron matrix (mf6)                    *
*     12           photon prod. xsec (photon yields given, mf12)   *
```

```
*     13           photon prod. xsec (photon xsecs given, mf13)   *
*     16           neutron-gamma matrix (photon yields given)     *
*     17           neutron-gamma matrix (photon xsecs given)      *
*     18           neutron-gamma matrix (mf6)                     *
*        note: if necessary, mfd=13 will automatically change    *
*        to 12 and mfd=16 will automatically change to 17 or 18.*
*     21           proton production matrix (mf6)                 *
*     22           deuteron production (mf6)                      *
*     23           triton production (mf6)                        *
*     24           he-3 production (mf6)                          *
*     25           alpha production (mf6)                         *
*     26           residual nucleus (a>4) production (mf6)        *
*     31           proton production matrix (mf4)                 *
*     32           deuteron production (mf4)                      *
*     33           triton production (mf4)                        *
*     34           he-3 production (mf4)                          *
*     35           alpha production (mf4)                         *
*     36           residual nucleus (a>4) production (mf4)        *
*          note: if necessary, mfd=21-26 will                     *
*          automatically change to 31-36.                         *
*     90+n         radioactive nuclide production from nth        *
*                   subsection for mtd in file 9.                 *
*    100+n         radioactive nuclide production from nth        *
*                   subsection for mtd in file 10.                *
*                                                                 *
*     mtd          meaning                                        *
*     ---          -------                                        *
*     -n           process all mt numbers from the previous       *
*                           entry to n inclusive                  *
*     221-250      reserved for thermal scattering                *
*     258          average lethargy                               *
*     259          average inverse velocity (m/sec)               *
*                                                                 *
*     automatic reaction processing options                       *
*     -------------------------------------                       *
*        3/        do all reactions in file3 on input pendf       *
*        6/        do all matrix reactions in endf dictionary     *
*       10/         do all radioactive isotope productions        *
*       13/        do all photon production cross sections        *
*       16/        do all photon production matrices              *
*       21/        do all proton production matrices              *
*       22/        do all deuteron production matrices            *
*       23/        do all triton production matrices              *
*       24/        do all he-3 production matrices                *
*       25/        do all alpha production matrices               *
*       26/        do all a>4 production matrices                 *
*                                                                 *
*******************************************************************
```

Input Instructions for GAMINR

```
*****************************************************************
*                                                               *
* card1                                                         *
*    nendf    unit for endf/b tape                              *
*    npend    unit for pendf tape                               *
*    ngam1    unit for input ngam tape (default=0)              *
*    ngam2    unit for output ngam tape (default=0)             *
* card2                                                         *
*    matb     material to be processed                          *
*             input materials in ascending order                *
*    igg      gamma group structure option                      *
*    iwt      weight function option                            *
*    lord     legendre order                                    *
*    iprint   print option (0/1=minimum/maximum) (default=1)    *
* card3                                                         *
*    title    run label up to 80 characters (delimited by *,    *
*             ended with /)                                     *
* card4       (igg=1 only)                                      *
*    ngg      number of groups                                  *
*    egg      ngg+1 group bounds (ev)                           *
* card5       (iwt=1 only)                                      *
*    wght     weight function as tab1 record                    *
* card6                                                         *
*    mfd      file to be processed                              *
*    mtd      section to be processed                           *
*    mtname   description of section to be processed            *
*             repeat for all reactions desired                  *
*             mfd=0/ terminates this material                   *
*             mfd=-1/ is a flag to process all sections present *
*             for this material  (termination is automatic)     *
* card7                                                         *
*    matd     next mat number to be processed                   *
*             terminate gaminr run with matd=0.                 *
*                                                               *
*---options for input variables----------------------------------*
*                                                               *
*         igg      meaning                                      *
*         ---      -------                                      *
*          0       none                                         *
*          1       arbitrary structure (read in)                *
*          2       csewg 94-group structure                     *
*          3       lanl 12-group structure                      *
*          4       steiner 21-group gamma-ray structure         *
*          5       straker 22-group structure                   *
*          6       lanl 48-group structure                      *
*          7       lanl 24-group structure                      *
*          8       vitamin-c 36-group structure                 *
*          9       vitamin-e 38-group structure                 *
*          10       vitamin-j 42-group structure                *
*                                                               *
*         iwt      meaning                                      *
*         ---      -------                                      *
*          1       read in                                      *
*          2       constant                                     *
*          3       1/e + rolloffs                               *
*                                                               *
*****************************************************************
```

Input Instructions for MODER

```
**********************************************************************
*                                                                    *
* card 1        unit numbers                                         *
*      nin      input unit                                           *
*      nout     output unit                                          *
*                                                                    *
*  a positive unit is coded (mode 3).                                *
*  a negative unit is blocked binary (njoy mode).                    *
*                                                                    *
*  note: abs(nin) ge 1 and le 19 is a flag to select various         *
*        materials from one or more input tapes, with or             *
*        without mode conversion.  the kind of data to be            *
*        processed is keyed to nin as follows:                       *
*             nin=1, for endf or pendf input and output,             *
*                 2, for gendf input and output,                     *
*                 3, for errorr-format input and output.             *
*                                                                    *
*      cards 2 and 3 for abs (nin) ge 1 and le 19 only.              *
*                                                                    *
* card 2                                                             *
*      tpid     tapeid for nout.  66 characters allowed              *
*               (delimited with *, ended with /)                     *
* card 3                                                             *
*      nin      input unit                                          *
*               terminate moder by setting nin=0                    *
*      matd     material on this tape to add to nout                *
**********************************************************************
```

Input Instructions for DTFR

```
*********************************************************************
*                                                                   *
* card 1        units                                               *
*    nin        input unit with data from groupr (binary).          *
*    nout       output unit containing dtf tables (coded).          *
*               (default=0=none)                                    *
*    npend      input unit with pendf tape for point plots.         *
*               (default=0=none)                                    *
*    nplot      output plot info for plotr module                   *
*               (default=0=none)                                    *
* card 2        options                                             *
*    iprint     print control (0 minimum, 1 maximum)                *
*    ifilm      film control (0/1/2=no/yes with 1 plot per frame/   *
*               yes with 4 plots per frame (default=0)              *
*    iedit      edit control (0/1=in table/separate) (default=0)    *
*                                                                   *
*       cards 3 through 5 only for iedit=0                          *
*                                                                   *
* card 3        neutron tables                                      *
*    nlmax      number of neutron tables desired.                   *
*    ng         number of neutron groups                            *
*    iptotl     position of total cross section                     *
*    ipingp     position of in-group scattering cross section.      *
*    itabl      neutron table length desired.                       *
*    ned        number of entries in edit table (default=0).        *
*    ntherm     number of thermal groups (default=0).               *
*  card 3a only for ntherm ne 0                                     *
* card 3a       thermal incoherent and coherent mts                 *
*    mti        mt for thermal incoherent data                      *
*    mtc        mt for thermal coherent data (default=0)            *
*    nlc        no. coherent legendre orders (default=0)            *
* card 4        edit names                                          *
*       six character hollerith names for edits for as many         *
*       cards as needed.  there will be iptotl-3 names read.        *
*       each name is delimited with *.                              *
* card 5        edit specifications                                 *
*       ned triplets of numbers on as many cards as needed.         *
*       positions can appear more than once.                        *
*       reaction types can appear more than once.                   *
*    jpos       position of edit quantity.                          *
*    mt         endf/b reaction number.                             *
*    mult       multiplicity to be used when adding this mt.        *
*                                                                   *
*       card 6 for iedit=1                                          *
*                                                                   *
* card 6        claw-format tables                                  *
*    nlmax      number of neutron tables (def=5)                    *
*    ng         number of neutron groups (def=30)                   *
*               (number of thermal groups is zero)                  *
*                                                                   *
* card 7        gamma ray tables                                    *
*    nptabl     number of gamma tables desired (default=0)          *
*    ngp        number of gamma groups (default=0)                  *
* card 8        material description                                *
*       one card for each table set desired.                        *
*       empty card (/) terminates execution of dtfr.                *
*    hisnam     6-character isotope name                            *
*    mat        material number as in endf/b (default=0)            *
*    jsigz      index number of sigma-zero desired (default=1)      *
*    dtemp      temperature desired (default=300)                   *
*                                                                   *
*********************************************************************
```

Input Instructions for MATXSR

```
*********************************************************************
*                                                                   *
* card 1 units                                                      *
*   ngen1      input unit for data from groupr                      *
*   ngen2      input unit for data from gaminr                      *
*   nmatx      output unit for matxs                                *
*   ngen3      incident proton data from groupr (default=0)         *
*   ngen4      incident deuteron data from groupr (default=0)       *
*   ngen5      incident triton data from groupr (default=0)         *
*   ngen6      incident he3 data from groupr (default=0)            *
*   ngen7      incident alpha data from groupr (default=0)          *
* card 2 user identification                                        *
*   ivers      file version number (default=0)                      *
*   huse       user id (up to 16 characters, delimited by *,        *
*              ended by /) (default=blank)                          *
* card 3 file control                                               *
*   npart      number of particles for which group                  *
*                 structures are given                              *
*   ntype      number of data types in set                          *
*   nholl      number of cards to be read for hollerith             *
*              identification record.                               *
*   nmat       number of materials desired                          *
* card 4 set hollerith identification                               *
*   hsetid     hollerith identification of set                      *
*              (each line can be up to 72 characters,               *
*              delimited with *, ended by /)                        *
* card 5 particle identifiers                                       *
*   hpart      hollerith identifiers for particles                  *
*              (up to 8 characters each)                            *
* card 6 energy groups                                              *
*   ngrp       number of groups for each particle                   *
* card 7 data type identifiers                                      *
*   htype      hollerith identifiers for data types                 *
*              (up to 8 characters each)                            *
* card 8 input particle ids                                         *
*   jinp     input particle id for each data type                   *
* card 9 output particle ids                                        *
*   joutp    output particle id for each data type                  *
* card 10 material data (one card per material)                     *
*   hmat       hollerith material identifier                        *
*              (up to 8 characters each)                            *
*   matno      integer material identifier                          *
*              (endf/b mat number)                                  *
*   matgg      mat number for photoatomic data                      *
*              (default=100*(matno/100) as in endf-6)               *
*                                                                   *
*********************************************************************
```

Input Instructions for ACER

```
**********************************************************************
*                                                                    *
* card 1                                                             *
*    nendf     unit for input endf/b tape                            *
*    npend     unit for input pendf tape                             *
*    ngend     unit for input multigroup photon data                 *
*    nace      unit for output ace tape                              *
*    ndir      unit for output mcnp directory                        *
* card 2                                                             *
*    iopt      type of acer run option                               *
*                1   fast data                                       *
*                2   thermal data                                    *
*                3   dosimetry data                                  *
*                4   photo-atomic data                               *
*                7   read type 1 ace files to print or edit          *
*                8   read type 2 ace files to print or edit          *
*                9   read type 3 ace files to print or edit          *
*    iprint    print control (0 min, 1 max, default=1)               *
*    ntype     ace output type (1, 2, or 3, default=1)               *
*    suff      id suffix for zaid (default=.00)                      *
*    nxtra     number of iz,aw pairs to read in (default=0)          *
* card 3                                                             *
*    hk        descriptive character string (70 char max)            *
*              delimited by quotes                                   *
* card 4 (nxtra.gt.0 only)                                           *
*    iz,aw     nxtra pairs of iz and aw                              *
*                                                                    *
*    --- fast data (iopt=1 only) ---                                 *
*                                                                    *
* card 5                                                             *
*    matd      material to be processed                              *
*    tempd     temperature desired (kelvin) (default=300)            *
* card 6                                                             *
*    err       tolerance for thinning distributions                  *
*    iopp      detailed photons (0=no, 1=yes, default=1)             *
* card 7                                                             *
*  type of thinning is determined by sign of thin(1)                 *
*  (pos. or zero/neg.=energy skip/integral fraction)                 *
*  (all entries defaulted=no thinning)                               *
*    thin(1)   e1 energy below which to use all energies (ev)        *
*              or iwtt weighting option (1=flat,2=1/e)               *
*              (1/e actually has weight=10 when e lt .1)             *
*    thin(2)   e2 energy above which to use all energies             *
*              or target number of points                            *
*    thin(3)   iskf skip factor--use every iskf-th energy            *
*              between e1 and e2, or rsigz reference sigma zero      *
*                                                                    *
*   --- thermal data (iopt=2 only) ---                               *
*                                                                    *
* card 8                                                             *
*    matd      material to be processed                              *
*    tempd     temperature desired (kelvin) (default=300)            *
*    tname     thermal zaid name ( 6 char max, def=za)               *
* card 8a                                                            *
*    iza01     moderator component za value                          *
*    iza02     moderator component za value (def=0)                  *
*    iza03     moderator component za value (def=0)                  *
* card 9                                                             *
*    mti       mt for thermal incoherent data                        *
*    nbint     number of bins for incoherent scattering              *
*    mte       mt for thermal elastic data                           *
*    ielas     0/1=coherent/incoherent elastic                       *
*    nmix      number of atom types in mixed moderator               *
*              (default=1, not mixed)                                *
*              (example, 2 for beo or c6h6)                          *
*    emax      maximum energy for thermal treatment (ev)             *
```

```
*              (default=1000.=determined from mf3, mti)          *
*     iwt      weighting option                                  *
*              0/1=variable/constant (default=variable)          *
*                                                                *
*    --- dosimetry data (iopt=3 only) ---                       *
*                                                                *
*  card 10                                                       *
*     matd     material to be processed                          *
*     tempd    temperature desired (kelvin) (default=300)        *
*                                                                *
*    --- photo-atomic data (iopt=4 only) ---                    *
*                                                                *
*  card 11                                                       *
*     matd     material to be processed                          *
*                                                                *
*    --- print or edit existing files (iopt=7-9) ---            *
*                                                                *
*     no additional input cards are required.  mount the old     *
*     ace tape on "npend".  the code can modify zaid, hk,        *
*     the (iz,aw) list, and the type of the file.  use suff<0    *
*     to leave the old zaid unchanged.  use just "/" on          *
*     card 3 to leave the comment field hk unchanged.  use       *
*     nxtra=0 to leave the old iz,aw list unchanged.             *
*     the code can modify zaid, hk, and type of file.            *
*                                                                *
*    exhaustive consistency checks are automatically made on     *
*    the input file.  if ngend.ne.0, a set of standard ace plots *
*    are prepared on unit ngend as plotr input instructions.     *
*                                                                *
******************************************************************
```

Input Instructions for WIMSR

```
************************************************************************
*                                                                      *
* card 1                                                               *
*    ngendf  unit for input gendf tape                                 *
*    nout    unit for output wims tape                                 *
*                                                                      *
* card 2                                                               *
*    iprint  print option                                              *
*               0=minimum (default)                                    *
*               1=regular                                              *
*               2=1+intermediate results                               *
*    iverw   wims version                                              *
*               4=wims-d (default)                                     *
*               5=wims-e                                               *
*    igroup  group option                                              *
*               0=69 groups (default)                                  *
*               9=user's choice                                        *
*                                                                      *
* card 2a  (igroup.eq.9 only)                                          *
*    ngnd    number of groups                                          *
*    nfg     number of fast groups                                     *
*    nrg     number of resonance groups                                *
*    igref   reference group (default is last fast group)              *
*                                                                      *
* card 3                                                               *
*    mat     endf mat number of the material to be processed           *
*    nfid    not used                                                  *
*    rdfid   identification of material for the wims library           *
*    iburn   burnup data option                                        *
*              -1=suppress printout of burnup data                     *
*               0=no burnup data is provided (default)                 *
*               1=burnup data is provided in cards 5 and 6             *
*                                                                      *
* card  4                                                              *
*    ntemp   no. of temperatures to process for this material          *
*            in the thermal energy range                               *
*               (0=all found on input tape)                            *
*    nsigz   no. of sigma zeroes to process for this material          *
*               (0=all found on input tape)                            *
*    sgref   reference sigma zero                                      *
*               (.ge. 1.e10 to select all cross sect. at inf.dil.      *
*                           but fully shielded elastic x-sect,         *
*                .lt. 1.e10 to select all x-sect at inf.dil.           *
*                =sig0      from the list on groupr input to           *
*                           select all x-sect. at that sig0)           *
*    ires    resonance absorber indicator                              *
*               0=no resonance tables                                  *
*              >0=ires temperatures processed                          *
*    sigp    potential cross section from endf/b.                      *
*               (if zero, replace by the elastic cross section)        *
*    mti     thermal inelastic mt (default=0=none)                     *
*    mtc     thermal elastic mt (default=0=none)                       *
*    ip1opt  include p1 matrices                                       *
*               0=yes                                                  *
*               1=no, correct p0 ingroups (default)                    *
*    inorf   resonance fission (if found)                              *
*               0=include resonance fission (default)                  *
*               1=do not include                                       *
*    isof    fission spectrum                                          *
*               0=do not include fission spectrum (default)            *
*               1=include fission spectrum                             *
*    ifprod  fission product flag                                      *
*               0=not a fission product (default)                      *
*               1=fission product, no resonance tables                 *
*               2=fission product, resonance tables                    *
*    jp1     transport correction neutron current spectrum flag        *
```

```
*               0=use p1-flux for transport correction (default)  *
*              >0=read in jp1 values of the neutron current       *
*                 spectrum from input                             *
*                                                                 *
*   following two cards are for iburn gt 0 only                   *
* card  5                                                         *
*    ntis    no. of time-dependent isotopes                       *
*    efiss   energy released per fission                          *
*                                                                 *
* card  6  (repeat this card ntis times)                          *
*    identa  ident of fission product isotope                     *
*    yield   fission yield of identa from burnup of mat           *
*                                                                 *
* card  7                                                         *
*    lambda  resonance-group goldstein lambdas (13 for            *
*            default 69-group structure, nrg otherwise).          *
*                                                                 *
* card  8    (only when jp1>0)                                    *
*    p1flx   current spectrum (jp1 entries read, the rest are     *
*            set with the default p1-flux calculated by njoy).    *
*                                                                 *
*******************************************************************
```

Input Instructions for PLOTR

```
*****************************************************************
*                                                               *
*  card 0                                                       *
*     nplt          unit for output plot commands               *
*     nplt0         unit for input plot commands                *
*                     default=0=none                            *
*                     output plot commands are appended         *
*                     to the input plot commands, if any.       *
*  card 1                                                       *
*     lori          page orientation (def=1)                    *
*                    0  portrait (7.5x10in)                     *
*                    1  landscape (10x7.5in)                    *
*     istyle        character style (def=2)                     *
*                     1 = roman                                 *
*                     2 = swiss                                 *
*     size          character size option                       *
*                     pos = height in page units                *
*                     neg = height as fraction of subplot size  *
*                     (default=0.30)                            *
*     ipcol         page color (def=white)                      *
*                    0=white                                    *
*                    1=navajo white                             *
*                    2=blanched almond                          *
*                    3=antique white                            *
*                    4=very pale yellow                         *
*                    5=very pale rose                           *
*                    6=very pale green                          *
*                    7=very pale blue                           *
*                                                               *
* -----repeat cards 2 through 13 for each curve-----            *
*                                                               *
*  card 2                                                       *
*     iplot         plot index                                  *
*                     99 = terminate plotting job               *
*                      1 = new axes, new page                   *
*                     -1 = new axes, existing page              *
*                      n = nth additional plot on existing axes *
*                     -n = start a new set of curves using      *
*                          the alternate y axis                 *
*                     default = 1                               *
*     iwcol         window color (def=white)                    *
*                    color list same as for ipcol above         *
*     factx         factor for energies (default=1.)            *
*     facty         factor for cross-sections (default=1.)      *
*     xll,yll       lower-left corner of plot area              *
*     ww,wh,wr      window width, height, and rotation angle    *
*                   (plot area defaults to one plot per page)   *
*                                                               *
* -----cards 3 thru 7 for iplot = 1 or -1 only-----             *
*                                                               *
*  card 3                                                       *
*     t1            first line of title                         *
*                   60 characters allowed.                      *
*                   default=none                                *
*                                                               *
*  card 3a                                                      *
*     t2            second line of title                        *
*                   60 characters allowed.                      *
*                   default=none                                *
*                                                               *
*  card 4                                                       *
*     itype         type for primary axes                       *
*                     1 = linear x - linear y                   *
*                     2 = linear x - log y                      *
*                     3 = log x - linear y                      *
*                     4 = log x - log y                         *
```

```
*                     set negative for 3d axes                    *
*                     default=4                                   *
*     jtype          type for alternate y axis or z axis          *
*                     0 = none                                    *
*                     1 = linear                                  *
*                     2 = log                                     *
*                     default=0                                   *
*     igrid          grid and tic mark control                    *
*                     0 = no grid lines or tic marks              *
*                     1 = grid lines                              *
*                     2 = tic marks on outside                    *
*                     3 = tic marks on inside                     *
*                     default=2                                   *
*     ileg           option to write a legend.                    *
*                     0 = none                                    *
*                     1 = write a legend block with upper left    *
*                         corner at xtag,ytag (see below)         *
*                     2 = use tag labels on each curve with       *
*                         a vector from the tag to the curve      *
*                     default=0                                   *
*     xtag           x coordinate of upper left corner            *
*                    of legend block                              *
*     ytag           y coord of upper left corner                 *
*                    default=upper left corner of plot            *
*                                                                 *
*  card 5                                                         *
*     el             lowest energy to be plotted                  *
*     eh             highest energy to be plotted                 *
*     xstep          x axis step                                  *
*                    default = automatic scales                   *
*                    (default all 3, or none)                     *
*                    (the actual value of xstep is                *
*                        ignored for log scales)                  *
*                                                                 *
*  card 5a                                                        *
*     xlabl          label for x axis                             *
*                    60 characters allowed.                       *
*                     default="energy (ev)"                       *
*                                                                 *
*  card 6                                                         *
*     yl             lowest value of y axis.                      *
*     yh             highest value of y axis.                     *
*     ystep          step for y ayis (linear scales only)         *
*                    default = automatic scales                   *
*                    (default all 3, or none)                     *
*                    (the actual value of ystep is                *
*                        ignored for log scales)                  *
*                                                                 *
*  card 6a                                                        *
*     ylabl          label for y axis                             *
*                    60 characters allowed.                       *
*                     default="cross section (barns)"             *
*                                                                 *
*  card 7   (jtype.gt.0 only)                                     *
*     rbot           lowest value of secondary y axis or z axis   *
*     rtop           highest value of secondary y axis or z axis  *
*     rstep          step for secondary y axis or z axis          *
*                    default for last three = automatic           *
*                                                                 *
*  card 7a  (jtype.gt.0 only)                                     *
*     rl             label for alternate y axis or z axis         *
*                    60 characters allowed.                       *
*                    default=blank                                *
*                                                                 *
*  -----cards 8 thru 9 are always given-----                      *
*                                                                 *
*  card 8                                                         *
*     iverf          version of endf tape                         *
*                      set to zero for data on input file         *
*                        and ignore rest of parameters on card    *
```

```
*                       set to 1 for gendf data                    *
*     nin             input tape                                   *
*                     can change for every curve if desired.       *
*     matd            desired material                             *
*     mfd             desired file                                 *
*     mtd             desired section                              *
*                      mtd=0 means loop over all reactions in mfd  *
*                      (usually one page per mt, but for mf=3,     *
*                      resonance reactions may have several pages) *
*     temper          temperature for endf/b data (k)              *
*                     default=0.                                   *
*     nth,ntp,nkh     see below (defaults=1)                       *
*                                                                  *
*       special meanings for nth,ntp,nkh for file 3 or 5 data      *
*            nth    number of subsection to plot                  *
*              (works for isomer prod, delayed n, etc.)          *
*            ntp    not used                                      *
*            nkh    not used                                      *
*                                                                  *
*       special meanings for nth,ntp,nkh for file 6 data           *
*            nth    index for  incident energy                    *
*            ntp    number of dep. variable in cyle to plot       *
*                   (or angle number for law 7)                   *
*            nkh    number of outgoing particle to plot           *
*                                                                  *
*       special meanings for nth,ntp,nkh for gendf mf=3 data       *
*            nth=0 for flux per unit lethargy                      *
*            nth=1 for cross section (default)                     *
*            ntp=1 for infinite dilution (default)                 *
*            ntp=2 for next lowest sigma-zero values, etc.         *
*            nkh=1 for p0 weighting (default)                      *
*            nkh=2 for p1 weighting (total only)                   *

*       special meaning for nth for gendf mf=6 data                *
*            nth=1 plot 2-d spectrum for group 1                   *
*            nth=2 plot 2-d spectrum for group 2                   *
*              etc.                                                *
*        no special flags are needed for mf=6 3d plots             *
*                                                                  *
*      special meanings for nth and ntp for mf7 plots              *
*           nth is index for indep. variable (alpha or beta)       *
*           ntp=1 selects alpha as indep. variable (default)       *
*           ntp=2 selects beta as indep. variable                  *
*           nkh=1 selects normal s(alpha,beta)                     *
*           nkh=2 selects script s(alpha,-beta)                    *
*           nkh=3 selects script s(alpha,beta)                     *
*                                                                  *
* -----cards 9 and 10 for 2d plots only-----                       *
*                                                                  *
*  card 9                                                          *
*     icon           symbol and connection option                 *
*                      0 = points connected, no symbols           *
*                     -i = points not connected, symbol at every   *
*                          ith point                               *
*                      i = points connected, symbol at every ith   *
*                          points                                  *
*                     default=0                                    *
*     isym           no. of symbol to be used                     *
*                      0 = square                                  *
*                      1 = octagon                                 *
*                      2 = triangle                                *
*                      3 = cross                                   *
*                      4 = ex                                      *
*                      5 = diamond                                 *
*                      6 = inverted triangle                       *
*                      7 = exed square                             *
*                      8 = crossed ex                              *
*                      9 = crossed diamond                         *
*                     10 = crossed octagon                         *
*                     11 = double triangle                         *
```

```
*                      12 = crossed square                              *
*                      13 = exed octagon                                *
*                      14 = triangle and square                         *
*                      15 = filled circle                               *
*                      16 = open circle                                 *
*                      17 = open square                                 *
*                      18 = filled square                               *
*                      default=0                                        *
*     idash           type of line to plot                             *
*                      0 = solid                                        *
*                      1 = dashed                                       *
*                      2 = chain dash                                   *
*                      3 = chain dot                                    *
*                      4 = dot                                          *
*                      default=0                                        *
*     iccol           curve color (def=black)                          *
*                      0=black                                          *
*                      1=red                                            *
*                      2=green                                          *
*                      3=blue                                           *
*                      4=magenta                                        *
*                      5=cyan                                           *
*                      6=brown                                          *
*                      7=purple                                         *
*     ithick          thickness of curve (def=1)                       *
*                      0 = invisible (for shaded areas)                 *
*     ishade          shade pattern                                    *
*                      0 = none                                         *
*                      1 to 10 = 10% to 100% gray                       *
*                      11 to 20 = 45 deg right hatching                 *
*                      21 to 30 = 45 deg left hatching                  *
*                      31 to 40 = 45 deg cross hatching                 *
*                      41 to 50 = shades of green                       *
*                      51 to 60 = shades of red                         *
*                      61 to 70 = shades of brown                       *
*                      71 to 80 = shades of blue                        *
*                      default=0                                        *
*                                                                       *
*  card 10  ---ileg.ne.0 only---                                       *
*     aleg            title for curve tag or legend block              *
*                     60 characters allowed.                           *
*                     default=blank                                    *
*                                                                       *
*  card 10a  ---ileg.eq.2 only---                                      *
*     xtag            x position of tag title                          *
*     ytag            y position of tag title                          *
*     xpoint          x coordinate of vector point                     *
*                      (.le.0 to omit vector)                          *
*                                                                       *
* -----card 11 for 3d plots only-----                                  *
*                                                                       *
*  card 11                                                             *
*     xv,yv,zv        abs. coords of view point                        *
*                     defaults=15.,-15.,15.                            *
*     x3,y3,z3        abs. sides of work box volume                    *
*                     defaults=2.5,6.5,2.5                             *
*                                                                       *
*          set x3 or y3 negative to flip the order of the               *
*          axis on that side of the work box.                           *
*                                                                       *
*  -----cards 12 thru 13 for iverf = 0 only-----                       *
*                                                                       *
*  card 12                                                             *
*     nform            format code for input data                      *
*                      0 = free format input with                      *
*                      optional x and y error bars                     *
*                                                                       *
*  card 13    ---nform = 0 only---                                     *
*     xdata            dependent value                                 *
*                      terminate with empty card (/)                   *
```

```
*     ydata          independent value                              *
*     yerr1          lower y error limit                            *
*                    no y error bar if zero                         *
*     yerr2          upper y error limit                            *
*                    if zero, equals yerr1                          *
*     xerr1          x left error limit                             *
*                    no x error bar if zero                         *
*     xerr2          x right error limit                            *
*                    if zero, equals xerr1                          *
*                                                                   *
*                                                                   *
* all curves contain at least 10 points per decade (see delta).    *
* code can plot curves containing fewer than 2000 points (see      *
* max) without thinning.  curves with more points are thinned       *
* based on a minimum spacing determined from max and the            *
* length of the x axis.                                             *
*                                                                   *
*********************************************************************
```

Input Instructions for VIEWR

```
**********************************************************************
*                                                                    *
* character specifications are similar to disspla, except that       *
* the default case is lower instead of upper.  this allows           *
* mixed-case strings to be used in postscript mode.  the             *
* following shift characters are used:                               *
*     < = upper-case standard                                        *
*     > = lower-case or mixed-case standard                          *
*     [ = upper-case greek                                           *
*     ] = lower-case or mixed-case greek                             *
*     # = instructions                                               *
* give one of the shift characters twice to get it instead of        *
* its action.  the following instructions are supported:             *
*     Ev = elevate by v as a fraction of the height                  *
*          if v is missing or D is given, use .5                     *
*     Lv = lower by v as a fraction of the height                    *
*          if v is missing or D is given, use .5                     *
*     Hv = change height by v as a fraction of the height            *
*          if v is missing or D is given, use .5                     *
*     Fi = change to font number i                                   *
*     Mi = change mode number, where mode 0 is the lower 128         *
*          postscript characters and mode 1 is the upper 128         *
*     X  = reset E, L, or H.  Font and Mode must be                  *
*          reset explicitly.                                         *
*     c is a real number, i is an integer.                           *
*                                                                    *
*---input-------------------------------------------------------------*
*                                                                    *
*  card 1                                                            *
*     infile         input file                                      *
*     nps            postscript output file                          *
*                                                                    *
*---data file format--------------------------------------------------*
*                                                                    *
*  card 1                                                            *
*     lori           page orientation (def=1)                        *
*                     0  portrait (7.5x10in)                         *
*                     1  landscape (10x7.5in)                        *
*     istyle         character style (def=2)                         *
*                       1  roman                                     *
*                       2  swiss                                     *
*     size           character size option                           *
*                       pos = height in page units                   *
*                       neg = height as fraction of subplot size     *
*                         (default=.30)                              *
*     ipcol          page color (def=white)                          *
*                     0=white                                        *
*                     1=navajo white                                 *
*                     2=blanched almond                              *
*                     3=antique white                                *
*                     4=very pale yellow                             *
*                     5=very pale rose                               *
*                     6=very pale green                              *
*                     7=very pale blue                               *
*                                                                    *
* -----repeat cards 2 through 13 for each curve-----                 *
*                                                                    *
*  card 2                                                            *
*     iplot          plot index                                      *
*                      99 = terminate plotting job                   *
*                       1 = new axes, new page                       *
*                      -1 = new axes, existing page                  *
*                       n = nth additional plot on existing axes     *
*                      -n = start a new set of curves using          *
*                           the alternate y axis                     *
*                      default = 1                                   *
```

```
*     iwcol          window color (def=white)                          *
*                     color list same as for ipcol above                *
*     factx          factor for energies (default=1.)                  *
*     facty          factor for cross-sections (default=1.)            *
*     xll,yll        lower-left corner of plot area                    *
*     ww,wh,wr       window width, height, and rotation angle          *
*                    (plot area defaults to one plot per page)         *
*                                                                      *
* -----cards 3 thru 7 for iplot = 1 or -1 only-----                    *
*                                                                      *
*  card 3                                                              *
*     t1             first line of title                               *
*                    60 characters allowed.                            *
*                    default=none                                      *
*                                                                      *
*  card 3a                                                             *
*     t2             second line of title                              *
*                    60 characters allowed.                            *
*                    default=none                                      *
*                                                                      *
*  card 4                                                              *
*     itype          type for primary axes                             *
*                      1 = linear x - linear y                         *
*                      2 = linear x - log y                            *
*                      3 = log x - linear y                            *
*                      4 = log x - log y                               *
*                      set negative for 3d axes                        *
*                      0 = no plot, titles only                        *
*                      default=4                                       *
*     jtype          type for alternate y axis or z axis               *
*                      0 = none                                        *
*                      1 = linear                                      *
*                      2 = log                                         *
*                      default=0                                       *
*     igrid          grid and tic mark control                         *
*                      0 = no grid lines or tic marks                  *
*                      1 = grid lines                                  *
*                      2 = tic marks on outside                        *
*                      3 = tic marks on inside                         *
*                      default=2                                       *
*     ileg           option to write a legend.                         *
*                      0 = none                                        *
*                      1 = write a legend block with upper left        *
*                          corner at xtag,ytag (see below)             *
*                      2 = use tag labels on each curve with           *
*                          a vector from the tag to the curve          *
*                      default=0                                       *
*     xtag           x coordinate of upper left corner                 *
*                    of legend block                                   *
*     ytag           y coord of upper left corner                      *
*                    default=upper left corner of plot                 *
*                                                                      *
*  card 5                                                              *
*     xmin           lowest energy to be plotted                       *
*     xmax           highest energy to be plotted                      *
*     xstep          x axis step                                       *
*                    default = automatic scales                        *
*                    (for linear, give all 3, or none)                 *
*                    (for log, give first 2, or none)                  *
*                                                                      *
*  card 5a                                                             *
*     xlabl          label for x axis                                  *
*                    60 characters allowed.                            *
*                    (default = no label, no numbering)                *
*                                                                      *
*  card 6                                                              *
*     ymin           lowest value of y axis.                           *
*     ymax           highest value of y axis.                          *
*     ystep          step for y ayis (linear scales only)              *
*                    default = automatic scales                        *
```

```
*                    (for linear, give all 3, or none)                  *
*                    (for log, give first 2, or none)                   *
*                                                                       *
*  card 6a                                                              *
*     ylabl          label for y axis                                   *
*                    60 characters allowed.                             *
*                    (default = no label, no numbering)                 *
*                                                                       *
*  card 7    (jtype.gt.0 only)                                          *
*     rmin           lowest value of secondary y axis or z axis         *
*     rmax           highest value of secondary y axis or z axis        *
*     rstep          step for secondary y axis or z axis                *
*                    (default = automatic scale)                        *
*                    (for linear, give all 3, or none)                  *
*                    (for log, give first 2, or none)                   *
*                                                                       *
*  card 7a   (jtype.gt.0 only)                                          *
*     rl             label for alternate y axis or z axis               *
*                    60 characters allowed.                             *
*                    (default = no label, no numbering)                 *
*                                                                       *
*   card 8   -- dummy input card for consistency with plotr             *
*                 it always should be 0/                                *
*                                                                       *
* -----cards 9 and 10 for 2d plots only-----                            *
*                                                                       *
*   card 9                                                              *
*     icon           symbol and connection option                       *
*                      0 = points connected, no symbols                 *
*                     -i = points not connected, symbol at every        *
*                          ith point                                    *
*                      i = points connected, symbol at every ith        *
*                          points                                       *
*                     default=0                                         *
*     isym           no. of symbol to be used                           *
*                      0 = square                                       *
*                      1 = octagon                                      *
*                      2 = triangle                                     *
*                      3 = cross                                        *
*                      4 = ex                                           *
*                      5 = diamond                                      *
*                      6 = inverted triangle                            *
*                      7 = exed square                                  *
*                      8 = crossed ex                                   *
*                      9 = crossed diamond                              *
*                     10 = crossed octagon                              *
*                     11 = double triangle                              *
*                     12 = crossed square                               *
*                     13 = exed octagon                                 *
*                     14 = triangle and square                          *
*                     15 = filled circle                                *
*                     16 = open circle                                  *
*                     17 = open square                                  *
*                     18 = filled square                                *
*                     19 = filled diamond                               *
*                     20 = filled triangle                              *
*                     21 = filled inverted triangle                     *
*                     22 = crossed circle                               *
*                     23 = exed circle                                  *
*                     24 = exed diamond                                 *
*                     default=0                                         *
*     idash          type of line to plot                               *
*                      0 = solid                                        *
*                      1 = dashed                                       *
*                      2 = chain dash                                   *
*                      3 = chain dot                                    *
*                      4 = dot                                          *
*                      5 = invisible                                    *
*                     default=0                                         *
*     iccol          curve color (def=black)                            *
```

```
*                    0=black                                          *
*                    1=red                                            *
*                    2=green                                          *
*                    3=blue                                           *
*                    4=magenta                                        *
*                    5=cyan                                           *
*                    6=brown                                          *
*                    7=purple                                         *
*     ithick        controls thickness of curve                      *
*                    0 = invisible (for shaded areas)                 *
*                    (default=1)                                      *
*     ishade        shade pattern                                    *
*                    0 = none                                         *
*                    1 to 10 = 10% to 100% gray                       *
*                    11 to 20 = 45 deg right hatching                 *
*                    21 to 30 = 45 deg left hatching                  *
*                    31 to 40 = 45 deg cross hatching                 *
*                    41 to 50 = shades of green                       *
*                    51 to 60 = shades of red                         *
*                    61 to 70 = shades of brown                       *
*                    71 to 80 = shades of blue                        *
*                    default=0                                        *
*                                                                     *
*   card 10    ---ileg.ne.0 only---                                   *
*     aleg          title for curve tag or legend block              *
*                   60 characters allowed.                           *
*                   default=blank                                    *
*                                                                     *
*   card 10a   ---ileg.eq.2 only---                                   *
*     xtag          x position of tag title                          *
*     ytag          y position of tag title                          *
*     xpoint        x coordinate of vector point                     *
*                    (.le.0 to omit vector)                          *
*                                                                     *
* -----card 11 for 3d plots only-----                                 *
*                                                                     *
*   card 11                                                           *
*     xv,yv,zv      abs. coords of view point                        *
*                   defaults= 15.,-15.,15.                           *
*     x3,y3,z3      abs. sides of work box volume                    *
*                   defaults=2.5,6.5,2.5                             *
*                                                                     *
*          set x3 negative to flip the order of the axis on         *
*          that side of the box (secondary energy, cosine).         *
*                                                                     *
*   card 12                                                           *
*     nform          format code for input data                      *
*                    0 = free format input with                      *
*                        optional x and y error bars                 *
*                    1 = free format input for a                     *
*                        3d family of curves z(x) vs y               *
*                                                                     *
*   card 13    ---nform = 0 only---   2-d data                        *
*     xdata          independent value                              *
*                    terminate with empty card (/)                  *
*     ydata          dependent value                                *
*     yerr1          lower y error limit                            *
*                    no y error bar if zero                         *
*     yerr2          upper y error limit                            *
*                    if zero, equals yerr1                          *
*     xerr1          x left error limit                             *
*                    no x error bar if zero                         *
*     xerr2          x right error limit                            *
*                    if zero, equals xerr1                          *
*                                                                   *
*   card 14    ---nform = 1 only---   3-d data                      *
*     y              y value for curve                            *
*                    repeat cards 13 and 13a for each curve       *
*                    terminate with empty card (/)                *
*                                                                 *
```

```
*    card14a    ---nform = 1 only---                                    *
*      x              x value                                          *
*      z              z value                                          *
*                     repeat card 13a for each point in curve          *
*                     terminate with empty card (/)                    *
*                     disspla version requires same x grid             *
*                     for each value of y.                             *
*                                                                      *
************************************************************************
```

Input Instructions for MIXR

```
**********************************************************************
*                                                                    *
*  card 1   --  units                                                *
*     nout       output unit for mixed cross sections               *
*     nin1       first input unit (endf or pendf)                   *
*     nin2       second input unit                                  *
*      ...        continue for nnin<=10 input units                 *
*                                                                    *
*  card 2   --  reaction list                                        *
*      mtn        list of nmt<=20 mt numbers for                    *
*                    the output reactions                            *
*                                                                    *
*  card 3   --  material list                                        *
*     matn,      list of nmat<=10 pairs (matn,wtn) of mat           *
*      wtn        numbers and associated weight factors             *
*                                                                    *
*  card 4   --  temperature                                          *
*     temp       temperature (use zero except for pendf tapes)      *
*                                                                    *
*  card 5   --  output material                                      *
*     matd       material number                                    *
*     za         za value                                           *
*     awr        awr value                                          *
*                                                                    *
*  card 6   --  file 1 comment card                                  *
*     des       description (60 char max)                           *
*                                                                    *
**********************************************************************
```

Input Instructions for LEAPR

```
**********************************************************************
*                                                                    *
* card 1 - units                                                     *
*    nout     endf output unit for thermal file                     *
*                                                                    *
* card 2 - title                                                     *
*                                                                    *
* card 3 - run control                                               *
*    ntempr  number of temperatures                                  *
*    iprint  print control (0=min, 1=more, 2=most, def=1)            *
*    nphon   phonon-expansion order (def=100)                        *
*                                                                    *
* card 4 - endf output control                                       *
*    mat     endf mat number                                         *
*    za      1000*z+a for principal scatterer                        *
*    isabt   sab type (0=s, 1=ss, def=0)                             *
*    ilog    log flag (0=s, 1=log10(s), def=0)                       *
*                                                                    *
* card 5 - principal scatterer control                               *
*    awr     weight ratio to neutron for principal scatterer         *
*    spr     free atom cross section for principal scatterer         *
*    npr     number of principal scattering atoms in compound        *
*    iel     coherent elastic option                                 *
*                  0  none (default)                                 *
*                  1  graphite                                       *
*                  2  beryllium                                      *
*                  3  beryllium oxide                                *
*    ncold   cold hydrogen option                                    *
*                  0   none (default)                                *
*                  1   ortho hydrogen                                *
*                  2   para hydrogen                                 *
*                  3   otho deuterium                                *
*                  4   para deuterium                                *
*                                                                    *
* card 6 - secondary scatterer control                               *
*    nss     number of secondary scatterers (0 or 1)                 *
*    b7      secondary scatterer type                                *
*             (0=sct only, 1=free, 2=diffusion)                      *
*    aws     weight ratio to neutron for secondary scatterer         *
*    sps     free atoms cross section for secondary scatterer        *
*    mss     number of atoms of this type in the compound            *
*                                                                    *
* card 7 - alpha, beta control                                       *
*    nalpha   number of alpha values                                 *
*    nbeta    number of beta values                                  *
*    lat      if lat.eq.1, alpha and beta values are scaled          *
*               by .0253/tev, where tev is temp in ev.  (def=0)      *
*                                                                    *
* card 8 - alpha values (increasing order)                           *
* card 9 - beta values (increasing order)                            *
*                                                                    *
* scatterer loop, do temperature loop for principal scatterer.       *
*         repeat for secondary scatterer (if any) if b7=0.           *
*                                                                    *
* temperature loop, repeat cards 10 to 18 for each temperature       *
*                                                                    *
*    card 10 - temperature (k)                                       *
*       a negative value means skip cards 11 to 18,                  *
*          thereby using previous parameters for this temp.          *
*                                                                    *
*    card 11 -- continuous distribution control                      *
*       delta    interval in ev                                      *
*       ni       number of points                                    *
*                                                                    *
*    card 12 -- rho(energy) (order of increasing ev)                 *
*                                                                    *
```

```
*     card 13 - continuous distribution parameters                    *
*        twt       translational weight                               *
*        c         diffusion constant (zero for free gas)             *
*        tbeta     normalization for continuous part                  *
*                                                                     *
*     card 14 - discrete oscillator control                           *
*        nd     number of discrete oscillators                        *
*                                                                     *
*     card 15 - oscillator energies (ev)                              *
*     card 16 - oscillator weights (sum to 1.-tbeta-twt)              *
*                                                                     *
*     card 17 - pair correlation control (ncold.ne.0 only)            *
*        nka     number of kappa values                               *
*        dka     kappa increment (inv. angstroms)                     *
*                                                                     *
*     card 18  skappa values in increasing order (inv. ang.)          *
*                                                                     *
* card 19 - file 1 comments, repeat until blank line is read.         *
*                                                                     *
***********************************************************************
```

Input Instructions for PURR

```
**********************************************************************
*                                                                    *
* card 1                                                             *
*   nendf   unit for endf/b tape                                     *
*   nin     unit for input pendf tape                                *
*   nout    unit for output pendf tape                               *
* card 2                                                             *
*   matd    material to be processed                                 *
*           matd=0 terminates purr                                   *
*   ntemp   no. of temperatures (10 max)                             *
*   nsigz   no of sigma zeros (10 max)                               *
*   nbin    no. of probability bins                                  *
*   nladr   no. of resonance ladders                                 *
*   iprint  print option (0=min, 1=max, def=1)                       *
*   nunx    no. of energy points desired (def=0=all)                 *
* card 3                                                             *
*   temp    temperatures in kelvin (including zero)                  *
* card 4                                                             *
*   sigz    sigma zero values (including infinity)                   *
*                                                                    *
**********************************************************************
```

Input Instructions for GASPR

```
************************************************************************
*                                                                      *
* card 1                                                               *
*    nendf    unit for endf/b tape                                     *
*    nin      unit for input pendf tape                                *
*    nout     unit for output pendf tape                               *
*                                                                      *
************************************************************************
```

Exercise 1: Linearization and Unionization

This exercise will make use of the RECONR module of NJOY to linearize the hydrogen cross sections to be accurate within a specified tolerance.

NJOY runs data through its various modules by using "tapes" to communicate between the modules (well, they are really files, except to the nostalgic). Therefore, NJOY input files give the module name to use, then the input and output units for that module, and then the characteristic input for that module. This is repeated for each module to be used, and then terminated with the module name "stop". Change to your NJOY working directory, and copy t511 to tape20. Type in the following input file (but leave off the comments to the right of the slash symbol):

```
reconr
20 21
'exercise 1'/     new tape ID title
1301 1/           MAT
.001/             fractional tolerance
'1-H-1'/          descriptive card for new tape
0/
stop
```

Save the file as in1.

This file says to run RECONR on MAT1301 with a reconstruction tolerance of .001 (.1%). The output will be on tape21. The title on the Tape ID card will be "exercise 1," and the single information line in the output file will say "1-H-1."

Run the NJOY job with this input file. Under unix or DOS, this can be done as follows:

```
xnjoy < in1
```

Examine the file called "output" to see the messages from RECONR. Examine the file called "tape21" to see what the new PENDF (pointwise ENDF) tape looks like.

- Check MF=3, MT=102 (radiative capture). Find the energies corresponding to energies on the original ENDF tape. Are the cross sections the same as the original ones?
- Look at the energies added by RECONR. Note the standard even values added, and also note where the intervals were divided in half for increased accuracy.
- What is the analytic shape of this radiative capture cross section at low energies? Where does it begin to deviate from this shape?
- What would the error have been at 1.5e-4 eV if linear interpolation had been used with the grid of the original ENDF tape?
- [*Optional*] Derive a formula for the energy grid spacing that would be required to achieve the fractional accuracy x for a $1/v$ cross section.
- Check MF=3, MT=2 (elastic scattering). Does the grid match the one found for MF=3, MT=102? What is the analytic shape of this cross section at low energies?
- Check MF=3, MT=1 (total cross section). Does the energy grid match those from the other sections? We call this the union grid. Are the cross section values really equal to the sum of the partial cross sections? This is one of the things that unionization makes possible.

NEXT INDEX

Exercise 2:
Broadening Simple Cross Sections

This exercise will make use of the BROADR module of NJOY to Doppler broaden the hydrogen cross sections and to demonstrate how simple cross section shapes change with temperature.

You should still be in your NJOY working directory, and t511 should still be copied to tape20. Edit your input file in1 to look like the following (but you can leave off the comments to the right of the slash symbol):

```
reconr
20 21
'exercise 2'/     new tape ID title
1301 1/           MAT
.001/             fractional tolerance
'1-H-1'/          descriptive card for new tape
0/
broadr
20 21 22
1301 1/           same MAT, one temperature
.001/             same tolerance
300./             broaden to 300K
0/
stop
```

Save the file as in2.

This file says to run RECONR on MAT1301 with a reconstruction tolerance of .001 (.1%). The output will be on tape21. The title on the Tape ID card will be "exercise 2," and the single information line in the output file will say "1-H-1." Then run the output of RECONR into BROADR (along with the original ENDF tape). Broaden the cross sections to 300K using .001 (.1%) as the linearization and unionization tolerance. The output is written on tape22.

Run the NJOY job with this input file.

Examine the file called "output" to see the new messages from BROADR. Examine the file called "tape22" to see what the new 300K PENDF tape looks like.

- Check MF=3, MT=102 (radiative capture). How have the cross sections changed with respect to those on the output file from RECONR (tape21)?
- Check MF=3, MT=2 (elastic scattering). How have the cross sections changed with respect to those on the output file from RECONR (tape21)?
- Check MF=3, MT=1 (total cross section). Is the energy grid still unionized? Are the cross section values really equal to the sum of the partial cross sections?

Change the temperature to 10000K and run the NJOY job again.

- Check MF=3, MT=102 (radiative capture). Have the cross sections changed very much?
- Check MF=3, MT=2 (elastic scattering). Have the cross sections changed? What do think the analytic shape of the cross section is after Doppler broadening?

NEXT INDEX

Exercise 3:
Resonance Reconstruction

This exercise will make use of the RECONR module of NJOY to reconstruct the resonance cross sections for Pu-238 and to examine the results for the first few resonances. Plotting of the cross sections will also be demonstrated.

Copy t404 from the NJOY distribution to tape20. This file contains the ENDF/B-IV version of the Pu-238 cross sections. Create a file named in3 containing the following lines (as usual, you can leave off the comments to the right of the slash symbol):

```
reconr
20 21
'exercise 3'/     new tape ID title
1050 1/           MAT
.001/             fractional tolerance
'94-Pu-238'/      descriptive card for new tape
0/
stop
```

This file says to run RECONR on MAT1050 with a reconstruction tolerance of .001 (.1%). The output will be on tape21. The title on the Tape ID card will be "exercise 3," and the single information line in the output file will say "94-Pu-238." The output is written on tape21.

Run the NJOY job with this input file.

Examine the file called "output" to see the new messages from BROADR. Note that 475 points were added for linearization even before resonance reconstruction began. The resolved resonance range is seen to run from 1 to 200 eV, and an additional 6215 points were added to represent the detailed shapes of the resonances. This particular evaluation uses the single-level Breit-Wigner resonance representation, which can produce negative elastic scattering cross sections, and the message from subroutine EMERGE indicates that that happened here.

Examine the file called "tape21" to see what the new resonance PENDF tape looks like.

- Check MF=3, MT=2 (elastic scattering). Find the lower limit of the resolved resonance range. What happens to the cross section there?
- Find the center of the lowest resonance at 2.855 eV. Note that the peak is at higher energies and that there is an interference dip at lower energies.
- Check the 18.56 eV resonance. Note the place where the interference minimum went negative and was replaced by a small number. This was one of the sources of the message from EMERGE. Note that the energy grid went to a precision of nine significant digits temporarily.
- Check MF=3, MT=102 (radiative capture). Where is the peak of the lowest resonance in this case?

- Check MF=3, MT=18 (fission cross section). Where is the peak of the lowest resonance in this case?

- Check MF=3, MT=1 (total cross section). Note that it is dominated by the capture component.

- Go back to the beginning of tape21 and look at File 1. Note the directory of sections--only Files 1, 2, and 3 are present. You can also see the Tape ID and comment lines from the input deck, and the third card shows a temperature of 0K and a reconstruction tolerance of 1e-3.

- Finally, scan down to MF2, MT152. This is a special NJOY section giving the infinitely dilute unresolved resonance range cross section. Note that the unresolved range runs from 200 eV to 10 keV.

Now, modify in3 to contain the following lines to enable the cross sections from tape21 to be plotted:

```
...

plotr
22/                 output file
/                   default page style
1/                  new axes, new curve
'94-Pu-238'/        title line 1
/                   no line 2 for titles
2/                  lin x - log y
1 5 1/              x-axis range and step
/                   default label
.1 1000/            y-axis range
/                   default label
4 21 1050 3 102/    data source for curve
/                   default curve style
2/                  second curve on axes
4 21 1050 3 2/      data source for curve
0 0 1/              dashed curve
3/                  third curve on axes
4 21 1050 3 18/     data source for curve
0 0 4/              dotted curve
99/                 finished
viewr
22 23/
stop
```

Run the NJOY job, and then use ghostview or any Postscript printer to look at the results on tape23. The solid curve is the capture cross section, the dashed curve is the weak elastic resonance, and the dotted line shows the weak fission resonance.

NEXT INDEX

$$PER = (25)\ \exp\ \{-0.25[\ell nY(A)]\} \qquad (4.1\text{–}1)$$

Estimated range of uncertainty: Y(A)/(1+PER/100) to Y(A)(1+PER/100)

Examples

Y(A), %	PER	1 + PER/100
10.	14.	1.14
1.	25.	1.25
0.1	44.	1.44
10^{-3}	141.	2.41
10^{-6}	791.	8.91
10^{-10}	7910.	80.10

As shown in the accompanying figures, most experimental chain yields fall within the estimated range of uncertainties (dotted lines), which suggests that most estimated chain yields, calculated from the equations below, should be reliable to within the estimated uncertainties.

The accompanying figures compare for a number of fission reactions the calculated curves (solid lines) and range of uncertainties (dotted lines) with experimental data (points). Contributions of individual Gaussian functions are also shown (dashed lines, etc.). Curves are shown both for the results of least squares calculations (labeled A and L.S. Parm.) and for results of calculations using systematic trends expressed in the equations below (labeled B and Sys. Parm.). As can be seen, the measured chain yields show fine structure that cannot be reproduced by sums of smooth Gaussian functions. Also, a number of the higher yields have been measured very accurately, to ~1%. These facts contribute to the reduced chi-square values being considerable greater than one. If the estimated model uncertainties, discussed above, are included as contributing errors in reduced chi-square calculations, the results are mostly less than one and are shown in parentheses in the figures.

Figures 4.1–2A,B, 4.1–4A,B, 4.1–5A,B, and 4.1–6A,B illustrate that complementary single Gaussian curves for each peak represent the experimental data reasonably well for high excitation energies and for $Z_F > 94$. The Gaussian functions for the large Z_F are modified to include an exponential decrease toward symmetry, as discussed above. The differences between the experimental data and the wings of the model curves for fission of californium isotopes, Figs. 4.1–5A,B and 4.1–6A,B, suggest that addition of a small Gaussian contribution to the wings could improve representation of experimental data by the model. This suggested model modification is illustrated in Figs. 4.1–3C, 4.1–4C, 4.1–5C, and 4.1–6C.

The mass distributions for the peaks from fission of thorium isotopes are quite narrow, and the central peaks are quite well resolved, as shown in Figs. 4.1–7A,B and 4.1–8A,B. The

Exercise 4:
Resonance Doppler Broadening

This exercise will make use of the RECONR and BROADR modules to reconstruct the resonance cross sections for Pu-238, broaden them to 10000K, and plot a comparison of the 0K and 10000K cross sections.

Copy t404 from the NJOY distribution to tape20. This file contains the ENDF/B-IV version of the Pu-238 cross sections. Create a file named in4 containing the following lines (as usual, you can leave off the comments to the right of the slash symbol):

```
reconr
20 21
'exercise 4'/     new tape ID title
1050 1/           MAT
.01/              fractional tolerance
'94-Pu-238'/      descriptive card for new tape
0/
broadr
20 21 22
1050 1/           MAT, one temperature
.01/              tolerance
10000/            temperature
0/
plotr
23/               output file
/                 default page style
1/                new axes, new curve
'94-Pu-238'/      title line 1
/                 no line 2 for titles
2/                lin x - log y
2 4 .5/           x-axis range and step
/                 default label
.1 1000/          y-axis range
/                 default label
4 21 1050 3 102 0./ data source for curve
1 3 0/            crosses with solid line
2/                second curve on axes
4 22 1050 3 102 10000./ data source for curve
0 0 1/            crosses with dashed curve
99/               finished
viewr
23 24/
stop
```

Run the NJOY job, and then use ghostview or any Postscript printer to look at the results on tape24. You can see how the Doppler broadening changed the sharp 0K resonance into the broader resonance appropriate to 10000K. We added crosses at the energy grid points to show how the grid is adjusted with temperature. Note the the grid points are very close together near the resonance energy for the 0K curve, and more widly spaced out on the shoulders of the curve. The broadened curve, on the other hand, has widely spaced points near the resonance energy, and the closely spaced points appear out on the steep descents at the "Doppler width."

Variations: change the energy range being plotted to 100 to 200 eV with steps of 20 eV. Change the reaction being plotted to elastic scattering. These graphs will look better if you take off the crosses (*e.g.*, use "0 0 0/" and "0 0 1/" for the curve styles).

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Exercise 5: Resonance Integrals

This exercise will make use of the RECONR and BROADR modules to reconstruct the resonance cross sections for U-235 and broaden them to 293.6K (.0253 eV). This will allow us to look at the standard thermal quantities computed by BROADR.

Copy t511 from the NJOY distribution to tape20. This file contains the ENDF/B-V version of the U-235 cross sections. Create a file named in5 containing the following lines (as usual, you can leave off the comments to the right of the slash symbol):

```
reconr
20 21
'exercise 5'/     new tape ID title
1395 1/           MAT
.002/             fractional tolerance
'92-U-235'/       descriptive card for new tape
0/
broadr
20 21 22
1395 1/           MAT, one temperature
.002/             tolerance
293.6/            temperature
0/
stop
```

Run the NJOY job, and then look at the resulting output file. Find the table labeled "thermal quantities at 293.6 K = .0253 eV." NJOY is often run at temperatures different than the one corresponding to .0253 eV, and this table is capable of showing values corresponding to both the temperature used (*e.g.*, 300K) and the standard value of .0253 eV. The table contains the simple fission and capture cross sections as evaluated at "tev" and .0253 eV, and it also contains the Maxwellian-weighted average of these cross sections ("thermal capture integral", "thermal fission integral"). For $1/v$ cross section shapes, these two numbers are proportional, and the "g-factor" listed is unity. For more general shapes, g-factors different from unity give a integral measure of how seriously the cross sections differ from the $1/v$ shape.

The "capture resonance integral" and the "fission resonance integral" give the integrated effect of the higher energy data.

The alpha, eta, and K1 integrals are commonly used in thermal reactor analysis.

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Exercise 6:
GROUPR Auto-Reaction Run

This exercise will make use of the RECONR and GROUPR modules to compute all the U-235 cross sections and matrices at zero Kelvin using the automatic reaction loop.

Copy t511 from the NJOY distribution to tape20. This file contains the ENDF/B-V version of the U-235 cross sections. Create a file named in6 containing the following lines (as usual, you can leave off the comments to the right of the slash symbol):

```
reconr
20 21
'exercise 6'/     new tape ID title
1395 1/           MAT
.002/             fractional tolerance
'92-U-235'/       descriptive card for new tape
0/
groupr
20 21 0 22
1395 1 0 5 1 1 1 1/
'exercise 6'/
0.
1e10
4/                a simple four-group structure
1.e-5 .624 1.e3 1.e6 10.e6
3/                do all cross sections
6/                do all matrices
0/
0/
stop
```

Run the NJOY job, and then look at the resulting output file. See what reactions show up for cross sections and matrices.

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Exercise 7: Cross Sections for WIMS

NJOY is most valuable when it makes data for code systems used for practical application calculations. As an example, we will use one of the NJOY standard test problems to prepare a WIMS library for Pu-239 from ENDF/B-IV. Here is a copy of the core part of in11 from the NJOY distribution:

```
moder
20 -21
reconr
-21 -22
'pendf tape for pu-238 from endf/b-iv tape 404'/
1050 3/
.005/
'94-pu-238 from endf/b tape t404'/
'processed by the njoy nuclear data processing system'/
'see original endf/b-iv tape for details of evaluation'/
0/
broadr
-21 -22 -23
1050 3 0 1 0 /
.005/
300. 900. 2100.
0/
unresr
-21 -23 -24
1050 3 7 1
300 900 2100
1.e10 1.e5 1.e4 1000. 100. 10. 1
0/
thermr
0 -24 -25
0 1050 8 3 1 0 1 221 0
300. 900. 2100.
.05 4.2
groupr
-21 -25 0 -26
1050 9 0 5 3 3 7 1
'94-pu-238'/
300. 900. 2100.
1.e10 1.e5 1.e4 1000. 100. 10. 1
3 1 'total'/
3 2 'elastic'/
3 16 'n2n'/
3 17 'n3n'/
3 18 'fission'/
3 102 'capture'/
3 221 'free gas thermal'/
6 2 'elastic'/
6 16 'n2n'/
6 17 'n,3n'/
6 18 'fission'/
6 51 'discrete inelastic'/
6 -59 'continued'/
6 91 'continuum inelastic'/
6 221 'free gas thermal'/
0/
3 1 'total'/
3 2 'elastic'/
3 18 'fission'/
3 102 'capture'/
```

```
3 221 'free gas thermal'/
6 2 'elastic'/
6 221 'free gas thermal'/
0/
3 1 'total'/
3 2 'elastic'/
3 18 'fission'/
3 102 'capture'/
3 221 'free gas thermal'/
6 2 'elastic'/
6 221 'free gas thermal'/
0/
0/
wimsr
-26 27
1/
1050 1 1050./
3 7 1e10 3 10.890 221 0/
1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1./
stop
```

Note that the THERMR module is run. Because WIMS is a thermal-reactor lattice code, it is important to include proper thermal cross sections. Also note that GROUPR requests self shielding. A careful treatment of resonance absorption is very important for doing good lattice calculations.

Run the job using a deck appropriate for your system.

Open the output file and scroll down to "wimsr". You will see a modified version of the GROUPR output. First, remember that WIMSR uses the conventional group ordering with group 1 being the high-energy group; GROUPR works backwards with group 1 being the low energy group. Since WIMS uses 69 groups, you can convert the group indices by subtracting from 70. You will find some other transformations: absorption is capture plus fission, and the scattering matrices have all the channels added together.

The "potential scattering cross section" of 10.89 in the input deck is obtained as $4\pi a^2$, where a is the scattering length from File 2 on the ENDF tape. It is important to include a nonzero value for this entry for resonance absorbers.

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