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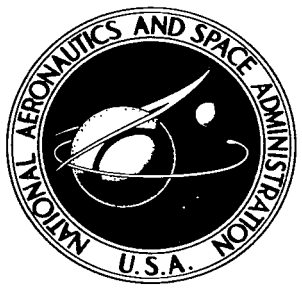

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A MONTE CARLO PROGRAM FOR CALCULATION OF DOPPLER COEFFICIENTS

by Robert E. Sullivan

Lewis Research Center
Cleveland, Ohio

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SUMMARY

A Monte Carlo program for the calculation of Doppler coefficients in arbitrary neutron flux spectra is presented. The program is designed to determine the effective cross sections of resonance scatterers and absorbers with a cylindrical or infinite slab geometry. The code may also be used to study the effect of resonance overlap in mixtures of isotopes and to investigate the approximations used in analytical calculations of the effective resonance integrals. As a test of the accuracy of the program, a flat in lethargy spectrum is used to obtain Doppler coefficients for several gold 197 samples, and the results are compared with values obtained by using the Nordheim calculation, which is expected to be nearly exact for such cases.

These calculations are compared with published experimental values of Doppler coefficients for gold 197. While a large discrepancy is observed between the Monte Carlo and experimental results, the Monte Carlo values agree well with the results of the Nordheim calculation.

INTRODUCTION

A Monte Carlo program is described that was developed to calculate reaction rates and Doppler coefficients for isotopic mixtures of resonance scatterers and absorbers with a cylindrical or infinite slab geometry. The basic quantity obtained from the Monte Carlo calculations is an "effective" cross section which, when multiplied by the integrated flux existing in the absence of the resonances, yields the correct reaction rate for the absorber. The ability to calculate this cross section in any given neutron flux spectrum is of importance in the study of temperature-dependent reactivity effects of nonthermal reactors. The code also permits the determination of effective cadmium cutoff energies and various activation ratios, as measured by threshold detectors.

The program evolved from a study of the application of Monte Carlo methods to the problem of detecting relatively small changes in reaction rate due to temperature varia-

tions. From the results obtained, it may be concluded that the method is capable of isolating these changes accurately.

The Monte Carlo method is not to be undertaken lightly since it requires much longer machine computation times than would an analytical program. Its use is justified only in situations where no complete analytical solution is available. Some of the factors affecting computation times are discussed briefly in the CONCLUSIONS section.

There are existing Monte Carlo codes which calculate resonance escape probabilities and capture rates, but these codes assume an asymptotic solution for the neutron slowing down density (refs. 1 and 2).

The present program was designed to solve the space- and energy-dependent problem for simple geometries while making as few approximations as possible. It allows the use of an arbitrary input neutron flux spectrum incident on, or distributed through, a sample consisting of up to five absorbing isotopes. The individual isotopic contributions to the reaction rate are separated so that resonance overlap effects may be evaluated. The program operation affords an accurate method for determining differences in reaction rate in parallel runs, as between two temperatures or for various isotropic mixtures, by forcing neutrons to follow identical histories to that point where the cases differ.

The type of Doppler experiment usually performed consists of a temperature-dependent activation or reactivity measurement on an absorber material inserted into a test region in which the unperturbed flux, or the flux exterior to the region, is known or may be calculated. Much of the experimental data available at present consists of measurements of effective resonance integrals and temperature coefficients in a neutron flux which is constant with lethargy in the absence of the absorber. The present Monte Carlo code has been used to calculate some of these experiments by generating this neutron flux at a boundary removed from the absorber test region.

There are analytical programs available which will calculate effective resonance integrals although they consider the resonances of mixtures of isotopes to be nonoverlapping (refs. 3 and 4), or consider the case of overlapping resonances for a $1/E$ neutron spectrum only (ref. 5). (All symbols are defined in appendix A.)

A test of the precision of the Monte Carlo code is the calculation of Doppler coefficients for an isotope such as gold, for which the analytic approximations should be valid. This test allows the Monte Carlo results to be compared with calculated results of the other programs (refs. 3 and 4) as well as with experiment.

The analysis section defines the basic quantities required and discusses some of the inherent differences in the analytical and experimental definitions of the fluxes used. A description of the manner in which individual neutron histories are traced is included along with the equations used in selecting neutron paths at points of interaction. The equations used in defining capture rates and resonance integrals in terms of the quantities computed by the code are also given.

The Monte Carlo results obtained for the Doppler coefficients of gold 197 are compared with values obtained by use of two of the analytical codes (refs. 3 and 4) currently in use as well as with experimental results.

Appendix B describes the input and output of the Monte Carlo program, outlines the method used in running problems which have the same geometry but varying cross sections, and demonstrates the manner in which the code may be used to solve certain classes of problems. Appendix C contains brief descriptions of the input and output for the programs used to generate and Doppler broaden nuclear cross sections for the Monte Carlo program. The method used in determining an optimum energy lattice for a given isotope is referenced, and listings of all codes are given in appendix D.

ANALYSIS

Definitions

In an activation calculation, the quantity desired is the number of neutron captures in each absorber isotope over the energy range specified for the problem. The reaction rate for a given process is the product of flux and cross section at all energies over the volume of interest and is given by

$$R = N_a \int_V \int_E \varphi_A(E, V)\sigma(E)dE\ dV \tag{1}$$

where φ_A is the actual flux existing in the sample. The effective cross section for an absorber occupying a finite volume is defined as

$$\sigma_{eff} \equiv \frac{\int_V \int_E \varphi_A(E, V)\sigma(E)dE\ dV}{\int_V \int_E \varphi_M(E, V)dE\ dV} \tag{2}$$

where the flux in the denominator is that which exists in the absence of the absorber. The correct reaction rate is then given by

$$R = N_a\sigma_{eff} \int_V \int_E \varphi_M(E, V)dE\ dV \tag{3}$$

The temperature coefficient may be defined in terms of the differences in reaction rate occasioned by temperature changes

$$\alpha(T_m) = \frac{2\left[R(T_2) - R(T_1)\right]}{(T_2 - T_1)\left[R(T_2) + R(T_1)\right]} \tag{4}$$

where the mean temperature T_m at which the coefficient obtains is taken to be

$$T_m = T_1 + \frac{1}{2}(T_2 - T_1) \tag{5}$$

These definitions may include, as a limiting case, the use of a neutron flux which is obtained from an asymptotic solution to the slowing down density. The flux in the absence of the absorber is then

$$\varphi_M(E) = \frac{q}{\xi N_s \sigma_s E} \tag{6}$$

and equation (1) becomes

$$R = \frac{qVN_a}{\xi N_s \sigma_s} \int_E \sigma(E) \frac{dE}{E}$$

The integral in this expression now corresponds to the usual definition of the "resonance integral" (ref. 6). This definition requires that the $1/E$ spectrum not be distorted by the absorber, which implies extreme dilution of the absorber. For noninfinitely dilute absorbers, the resonance integral must be redefined to allow for arbitrary deviations from the assumed $1/E$ flux spectrum. The effective resonance integral is, from reference 7, "the lethargy integral of that cross-section which, when multiplied by the flux which would exist in the absence of the resonance, would give the true absorption rate."

The effective cross section defined by equation (2), modified to include the neutron spectrum of equation (6), then yields the effective resonance integral when integrated over lethargy

$$I_{eff} = \sigma_{eff} \int_u du = \frac{\xi N_s \sigma_s}{qV} \int_V \int_E \varphi_A(E, V)\sigma(E)dE\, dV \tag{8}$$

A given experiment for the determination of the effective resonance integral generally consists of placing the absorber, surrounded by a cadmium cover, into a moderator region in which the neutron flux, in the absence of the absorber, is approximately uniform in space and lethargy. Experimentally, the flux in the absence of the resonances cannot be measured, and the flux must be that which exists when only the absorber potential scattering is used or when the absorber is replaced with moderator. Either of these fluxes may be used in the present program. The flux incident on the absorber may be presumed to be inversely proportional to the neutron energy, but this is not strictly correct as the absorber may perturb the flux exterior to its surface (ref. 8). Analytically, the limits on the lethargy integral, as defined previously, are taken to be from 0.4 electron volt (0.64×10^{-19} J) (the nominal cadmium cutoff energy) to infinity. However, as the position of the cadmium cutoff may affect the value of the integral, it is necessary to determine this energy accurately for each configuration. The infinite upper limit may be replaced by an energy beyond which the absorption rate increases by a negligible amount.

If equation (8) is used to obtain the effective resonance integral of an absorber at two temperatures, the temperature coefficient for that absorber may be calculated in terms of the I_{eff} for suitably small increments in absorber temperature T as

$$\alpha T_m = \frac{2\left[I_{eff}(T_2) - I_{eff}(T_1)\right]}{(T_2 - T_1)\left[I_{eff}(T_2) + I_{eff}(T_1)\right]} \tag{9}$$

since

$$I_{eff} = \frac{R\int_u du}{N_a \int_V \int_E \varphi_M(E, V)dE\, dV} = \text{Constant} \times R \tag{10}$$

This temperature coefficient comprises two major effects, the Doppler broadening due to a variation in relative velocity of the neutron and target nucleus and that occasioned by a change in the geometric size of the sample. The relative importance of the two effects may vary greatly and is dependent on the resonance structure and flux spectrum used. In the determination of effective resonance integrals for the isotope studied in this report, where a 1/E neutron flux spectrum is specified, only that component of the temperature coefficient due to Doppler broadening is important, and the temperature coefficient may be replaced by the Doppler coefficient, α_D, as defined in equation (9).

Monte Carlo Procedure

The Monte Carlo procedure may be applied so that resonance integrals and, consequently, Doppler coefficients may be calculated. The geometry and composition of absorber selected may be related to specific experiments. It is assumed that there exists a test region, which normally contains moderator material, at the outer boundary of which the neutron flux is isotropic and uniform in space and lethargy. An absorber sample, clad in cadmium is placed into this test region. The test region is large enough so that the flux at the outer boundary is not perturbed. Neutrons from the incident distribution are then traced through the test region until they are absorbed, moderated, or until they escape. Tabulations by energy interval and for each isotope in the absorber are made of absorptions and reaction rates for all neutrons entering the absorber. The sum of the reaction rates for neutrons of all energies within the absorber volume is the total reaction rate. This quantity, divided by the absorber atomic density and the integrated flux in the absence of the absorber, multiplied by the lethargy integral, is the effective resonance integral, as defined in equation (8). The flux in the absence of the absorber is determined by running the program with an identical geometry but with moderator or absorber potential scattering replacing the absorber cross sections.

Although the Monte Carlo code is adaptable to other geometries, the version presented in this report is restricted to concentric, finite cylinders within the test region. The test region is a surrounding region with planar boundaries, generally containing moderator material, and furnishes the surface on which the flux is prescribed. In order to analyze samples whose surface-to-mass ratios approach that of the infinitely dilute case, the cylindrical geometry must approach the shape of either a wire or a thin foil. In either of these cases, the statistical variance may be greatly increased due to large contributions to the reaction rate made by neutrons traveling in the direction parallel to the larger cylinder dimension. As most experiments use thin foils, a provision has been made in the present program to run the foil and investigate only that component of the results perpendicular to the foil surface.

Neutron Tracking

A brief outline of the methods and equations used in generating and tracking neutrons is presented. The subroutines are described in the order normally encountered in the execution of the program.

INIPOS. - The initial position of the neutron is first specified. As the neutron spatial density is uniform, the relative frequency with which neutrons appear on a particular face is proportional to the ratio of the area of that face to the total area of the outer

boundary surface. By comparing area ratios with a random number, an initial face is chosen. The remaining coordinates are then determined depending on the geometry. For a rectangle, for example, if $\mathcal{R}$ is a random number,

$$\frac{A_x + A_y}{A_T} < \mathcal{R} \leq \frac{A_x + A_y + A_z}{A_T}$$

places the neutron on the Z surface. The x- and y-coordinates are then chosen by random number

$$x = X(1 - 2\mathcal{R})$$

$$y = Y(1 - 2\mathcal{R})$$

Each coordinate is allowed to assume any value over its full range (i.e., $-X \leq x \leq X$). By altering the conditions on the position coordinates, the neutron flux may easily be placed throughout the test region rather than restrained to the boundaries.

ESTART. - The initial neutron energy is now determined. The number of neutrons that has a particular energy is inversely proportional to that energy. The equation used is such that each random number returns an energy with the proper relative frequency,

$$E_s = E_l \exp\left(\mathcal{R} \ln \frac{E_h}{E_l}\right)$$

and, in the limits $0 \leq \mathcal{R} \leq 1$, the allowed energy range is that specified for the problem. Any arbitrary energy spectrum may be used by changing the preceding equation.

ISOTRO. - Direction cosines for the neutron are assumed to be isotropic in the laboratory system for the initial flight. In order to avoid tracking neutrons beyond the outer boundary planes, the initial direction cosines are chosen to force the neutron into the test region. For example, for an initial position on the positive Z-face,

$$\omega_z < 0$$

indicates motion toward the cylinder.

CMLAB. - All collisions subsequent to the first are isotropic in the center-of-mass system. This subroutine uses the standard equations (ref. 9) to find the energy and direction cosines in the laboratory system based on isotropic scattering in the center-of-mass system.

SIGM. - The neutron may travel in any of several regions. In the code, all regions other than that occupied by the absorbers are considered to contain only one material. This subroutine finds the cross sections in any of the outer regions by interpolating between input table values.

SIGA. - In the absorber region, several isotopes may be present. Subroutine SIGA finds the cross sections for each isotope in the same manner as SIGM and also computes the total microscopic cross sections for the absorber.

ISOPIK. - In the absorber region, the isotope with which a neutron interacts is determined by the ratio of the macroscopic cross section of that isotope to the total macroscopic cross section. If

$$\mathcal{R} \leq \frac{\Sigma_T^1 + \Sigma_T^2 + \ldots + \Sigma_T^I}{\Sigma_T}$$

the interaction is with the isotope I.

MFP. - The distance D to be traveled by a neutron in the absence of any interaction with a boundary is then selected by a random choice of the number of mean free paths in the medium:

$$D = \frac{-\ln \mathcal{R}}{\Sigma_T}$$

CYLTCK. - The shortest distance to a geometric interaction is determined by this subroutine. The equations governing intersection of a directed line with a cylindrical surface (ref. 10) are used to determine whether a boundary is crossed before the nuclear collision occurs. If so, the direction cosines and energy of the neutron are unchanged but a new distance to nuclear interaction is chosen for the material occupying the new region. If the nuclear interaction takes precedence, the choice between scattering and absorption is made by comparing

$$R \leq \frac{\Sigma_s}{\Sigma_T}$$

If true, the neutron is scattered; if not, it is absorbed.

XOYOZO. - When the shortest distance to interaction is determined, the neutron is positioned at the correct point by use of the equations

$$x_2 = x_1 + \omega_x D$$

$$y_2 = y_1 + \omega_y D$$

$$z_2 = z_1 + \omega_z D$$

and tested to determine if it has escaped from the test region. If not, the entire process is repeated until the neutron is absorbed, moderated, or until it escapes.

DOPPLER COEFFICIENTS FOR GOLD 197

In order to test the precision of the Monte Carlo program in calculating the relatively small differences in reaction rate caused by the Doppler effect, a flat in lethargy neutron flux spectrum has been used to evaluate the Doppler coefficients of several gold samples ranging in square root of surface to mass ratio $\sqrt{S/M}$ from 1 to 50. These coefficients were calculated by using equations (8) and (9).

The use of an absorber consisting of a single isotope in a flux which is inversely proportional to the neutron energy allows the Monte Carlo results to be compared with values obtained from the Nordheim calculation (ref. 3), which is expected to be nearly exact in such cases. In addition, some preliminary experimental temperature coefficients (refs. 11 and 12) are available for comparison. The resonance parameters used in the analysis were those measured by Desjardins, et al. (ref. 13) with the BWSL (Breit-Wigner Single Level) and DBCS (Doppler Broadened Cross Sections) programs (described in appendix C) used to generate Doppler broadened cross sections for the Monte Carlo code. The experiments referenced were performed on gold foils at temperatures between 295° and 575° K, while the calculations were for foils at 295° and 543° K. As the Doppler coefficient is a slowly varying function of temperature, this comparison should be valid. The measured reaction rates were used directly, in accord with equation (4)

$$\alpha_D = \frac{2\left[R(T_2) - R(T_1)\right]}{(T_2 - T_1)\left[R(T_2) + R(T_1)\right]}$$

to evaluate the Doppler coefficient and, therefore, no direct value of the effective resonance integrals for these measurements is given. The experimental error is quoted at about 12 percent.

The results for all methods are given numerically in table I, which presents calculated and experimental values of the Doppler coefficient as a function of the $\sqrt{S/M}$. As

the Doppler coefficient depends on the normalizing value of the effective resonance integral, consistent values, as measured by the author of the experimental Doppler coefficients, of the effective resonance integral (ref. 14) were used. These values are also presented in table I.

Figure 1 presents curves of the Doppler coefficient as a function of the $\sqrt{S/M}$. The solid line represents values obtained by the Nordheim calculation with the Monte Carlo and experimental values also shown.

The agreement with experiment, as demonstrated in this figure, is poor. Phenomenologically, it may be expected that the Doppler coefficient curve for gold should have a peak, at some relatively high value of the $\sqrt{S/M}$, caused by self-shielding of the large first gold resonance, and then rise gradually as the effect of remaining higher energy resonances becomes predominant. The experimental measurements suggest only a slight variation with surface to mass ratio and agree reasonably well with the Monte Carlo results only at lower $\sqrt{S/M}$ values. In an attempt to determine whether the disagreement was in the Monte Carlo calculation, the quantities ΔI_{eff} and α_D were calculated by using the analytical code ZUT cited in reference 3. The Nordheim calculation, on which this code is based, is expected to give accurate results under the stated assumptions. Values of the Doppler coefficient calculated by the analytical code TRIX (ref. 12) were also compared with the Monte Carlo and ZUT results. As the ZUT and TRIX codes use similar analytic approximations, their results for α_D should be consistent. They do not, however, agree as the TRIX results are consistently lower than the ZUT values which are intermediate to, but in better agreement with, the Monte Carlo calculations. In addition, although the peak in the Doppler coefficient curve occurs at roughly the same surface to mass ratio for all methods, the TRIX peak in ΔI_{eff} is at a higher $\sqrt{S/M}$ ratio than indicated by the Monte Carlo and ZUT results.

Nearly all the discrepancy between the Monte Carlo and the Nordheim method (ZUT) is attributable to the small differences in Doppler broadened input cross sections used. The ZUT program, when run at a surface to mass ratio corresponding to infinite dilution, yields a Doppler coefficient of approximately zero. The codes used to prepare the Monte Carlo cross sections show an increase of 2 barns (2×10^{-24} cm^2) in the infinitely dilute resonance integral, nearly all of which occurs in the 4.906-electron-volt (7.86×10^{-19}-J) resonance. While the infinitely dilute values would be expected to vary with temperature due to weighting with a nonsymmetrical 1/E flux, the magnitude of the change is small and depends strongly on the energy intervals used in the numerical integration but infers a nonzero infinitely dilute Doppler coefficient. A previously reported change of 0.7 barn (0.7×10^{-24} cm^2) in 1580 barns (1.58×10^{-21} cm^2) for I_{eff} of gold between absolute zero and room temperature has been calculated elsewhere (ref. 15). This increase in the infinitely dilute integral is of importance as it is retained for the thicker samples and is one of the causes for the higher Doppler values obtained by the Monte Carlo code. In

order to verify this, the cross sections used in ZUT for the gold resonance at 4.906 electron volts (7.86×10^{-19} J) were run in the Monte Carlo code at surface to mass ratios for which the entire Doppler coefficient is a result of this resonance. Comparison of these results, at the $\sqrt{S/M}$ values indicated in table II, shows that both effective resonance integrals and Doppler coefficients are in close agreement. As the effect of this resonance is less pronounced in the thicker samples, the Monte Carlo and ZUT results, as indicated in figure 1 and table I, are in better agreement for the other surface to mass ratios investigated even though the cross-section sets used in these two codes differ slightly. The results of the Monte Carlo program conform to the shape of the Doppler coefficient curve predicted by the analytical code and agree to within about 10 percent with the predicted numerical values.

The differences between the calculated and experimental results are more difficult to explain. They are not a result of incorrect cross sections since the most pronounced discrepancies occur at surface to mass ratios where the Doppler coefficient is dominated by the large first resonance for which the parameters are well documented.

CONCLUSIONS

The Monte Carlo method outlined in this report is capable of accurately calculating small differences in the reaction rate of absorptive samples resulting from a given change in temperature. This was demonstrated by using a flat in lethargy neutron flux spectrum to calculate Doppler coefficients for a wide range of gold samples. The use of this flux spectrum and an absorber which conforms to the approximations required by the Nordheim calculation has allowed the Monte Carlo results for the Doppler coefficients to be compared with those obtained from an existing analytical code (ZUT) which is known to yield valid results.

The published experimental Doppler measurements exhibit little agreement with either the ZUT or Monte Carlo results. The absence of any variation in the experimental Doppler coefficient, particularly at surface to mass ratios for which a maximum in this function is predicted by both the Monte Carlo and Nordheim calculations, would tend to indicate that the experimental measurements should be reevaluated.

The major disadvantage of the Monte Carlo method is, of course, the large amount of machine time required. The running time is a function of the number of resonance levels which must be statistically sampled for a given absorber surface to mass ratio and of the probable error allowed. While integral quantities, such as reaction rates, may be obtained in from 5 to 15 minutes for the range of surface to mass ratios investigated in this report, the need for extreme accuracy in determining temperature effects

requires runs of the order of 15 to 60 minutes for the determination of Doppler coefficients on an IBM 7094 computer.

The primary advantage of the Monte Carlo method is its flexibility in studying effects such as resonance overlap in mixtures of isotopes. The complete solution of the space and energy dependent problem in an arbitrary neutron spectrum does not appear to be feasible by any other method.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, July 20, 1967,
120-27-06-18-22.

APPENDIX A

SYMBOLS

A	area, cm^2
A_T	total surface area, cm^2
D	distance to any interaction, cm
E	energy, eV; J
E_h	upper energy limit, eV; J
E_ℓ	lower energy limit, eV; J
E_s	initial energy, eV; J
I_{eff}	effective resonance integral, b; cm
ΔI_{eff}	change in effective resonance integral
N	total number of neutrons in problem
N_a	absorber atomic density, atoms/cm^3
N_s	moderator atomic density, atoms/cm^3
P.E.	probable error
q	slowing down density, neutrons/(cm^3)(sec)
R	reactions
$\mathcal{R}$	random number
T	temperature, ^oK
TL	track length, cm
T_m	mean temperature, ^oK
u	lethargy
V	volume, cm^3
X, Y, Z	initial (surface) coordinates, cm
x, y, z	Cartesian coordinates, cm
α	temperature coefficient, $(^oK)^{-1}$
α_D	Doppler coefficient, $(^oK)^{-1}$
ξ	average logarithmic decrement
Σ_s	macroscopic scattering cross section, cm^{-1}
Σ_T	macroscopic total cross section for region, cm^{-1}
Σ_T^i	macroscopic total cross section for isotope, cm^{-1}
σ	microscopic cross section, cm^2
σ_{eff}	effective cross section, cm^2
σ_s	microscopic scattering cross section, cm^2
φ_A	neutron flux in absorber, neutrons/(cm^2)(sec)
φ_M	neutron flux in moderator, neutrons/(cm^2)(sec)
$\omega_x, \omega_y, \omega_z$	direction cosines for x-, y-, and z-directions

APPENDIX B

MONTE CARLO CODE INPUT AND OUTPUT

The input and output for the Monte Carlo program is described. These may vary slightly for different versions of the code and the order listed corresponds to the version in appendix D.

Input

Card	Quantity	Format	Card columns	Remarks
1	EH	E12.5	1-12	Upper energy limit
	EL	E12.5	13-24	Lower energy limit
	XCAP	E12.5	25-36	Half dimensions of outer boundary in x-, y-, and z-directions
	YCAP	E12.5	37-48	
	ZCAP	E12.5	49-60	
2	NHIST	I6	1-6	Number of neutron histories
	MIST	I6	7-12	Internal mechanism for running more than 32 767 histories; use any integer less than this

In each standard case, the number of outer loops run is printed out. In subsequent parallel runs, MIST is not used directly but must have a value such that NHIST/MIST equals the number of outer loops.

NREG	I6	13-18	Number of zones
NISO	I6	19-24	Number of elements or isotopes in absorber
IGRP	I6	25-30	To minimize search time in cross section tables, only each IGRPth energy is tested until neutron energy is bracketed
INTER	I6	31-36	Number of neutron histories processed between time checks
NG	I6	37-42	Number of energy groups
PHIBAS	E12.5	43-54	Flux in absence of absorber; may be determined in prior run with moderator only present

Card	Quantity	Format	Card columns	Remarks
2	TEND	E12.5	55-66	Machine time; checked every INTER neutrons and final edit performed when actual machine time exceeds TEND
3	RCYL(I)	E12.5	1-12	Radius and half-height of concentric cylinders.
	H(I)	E12.5	13-24	Innermost first with three sets per card.
4	N(I)	E12.5	1-12	Final energy lattice number, abundance weighted
	D(I)	E12.5	13-24	nuclear density, and isotopic mass of each
	A(I)	E12.5	25-36	material; one set per card
5	EG(I)	6E12.5	1-72	NG+1 energies bounding NG groups in descending order
6	E(I)			Beginning with first isotope in absorber and con-
	S(I)			tinuing through last zone, and energies, scatter-
	T(I)			ing, and total cross sections

The energies and cross sections are normally read in binary form, in descending order. In this case, all energies are first read in, then all scattering cross sections, and, last, all total cross sections. Internally, each set of E, S, and T is used with no distinction made for different isotopes or materials; that is, if the number of the last E, S, and T for the first isotope is i (so that N(1) = i), the first set for the next isotope is i + 1. The program differentiates between cross-section sets only by the final energy lattice number N(I) which must be correct.

Decimal cards may be used to read in the cross-section sets if the three BCREAD statements in the main program are replaced by:

```
READ (5, 510) (E(I), S(I), T(I), I = M1, NN)

510 FORMAT(1P3E12.5)
```

7	MATCH	I3	1-3	Parallel run restart control; yes = 1; no = 0
	LRN	012	4-15	First random number constant if new case is run; usually 000000000001

The pseudorandom numbers generated by the program are controlled by an octal constant, LRN; that is, if a given LRN is used to begin generating a series of random numbers, this series will be duplicated each time that LRN is used as a lead constant. Most temperature dependent experiments consist of measurements made on a given external configuration with, theoretically, only the absorber temperature varying. In such cases, the random numbers controlling the neutron path would be temperature independent until the neutron entered the absorber and then until the neutron encountered a cross-section set changed by the Doppler broadening. The program contains an option for storing on tape the lead LRN for each neutron which entered the absorber. The use of these numbers to "restart" neutrons in cases which differ only slightly from the original case allows the perturbations to be calculated more accurately. The same method may be used when a series of absorbers of the same size but different isotopic compositions are compared.

The LLRN(LAT) are these octal restart numbers. They are written out on tape for all runs made with MATCH = 0 and NPCH = 1. If MATCH = 1 and the tape is mounted on unit 1, the restart case will be run.

Card	Quantity	Format		Remarks
7	NPCH	I3	16-18	Tape storage of random number constants; store = 1; no tape = 0
	KSLB	I3	18-21	Infinite slab control; yes = 1; no = 0

Output

The program output is, in general, sufficiently well described by the printed headings. Some aspects of certain output quantities are discussed to define them more precisely and enable the user to evaluate the results better.

The fundamental quantity evaluated by the program is the neutron flux. The sum of the track lengths of neutrons of all energies in a given volume V is the integrated flux (ref. 16)

$$\int_V \int_E \varphi(E, V)dE\ dV = \sum_{E,V} TL \tag{B1}$$

When the integrated flux is normalized by the total number of neutrons N entering the volume, the result is an average track per neutron $\overline{TL}$ in the volume, and it is this quantity which is printed out by the program.

To use equation (2), the integrated reaction rate in V, in accord with the definition

in equation (B1), is taken to be

$$\sum_{N} TL(E)N_a\sigma(E) = \int_V \int_E \varphi(E, V)N_a\sigma(E)dE\ dV \tag{B2}$$

To find the correct σ_{eff}, this quantity must be divided by the integrated flux, in the absence of the absorber, produced by the same number of neutrons traced in equation (B2). To accomplish this, the quantity in equation (B2) is divided by the average track length per neutron in the absence of the absorber $\overline{TL_M}$ multiplied by the number of neutrons run; that is,

$$\sigma_{eff} = \frac{\sum_{N} TL(E)\sigma(E)}{N\overline{TL_M}} \tag{B3}$$

This result, when multiplied by the lethargy integral, is the effective resonance integral.

As the reaction rates and absorptions are separated by isotope in the program, the absorptions, the square root of the surface to mass ratio, and effective resonance integrals for the individual isotopes are returned by the program. It should be remembered that these absorptions, reaction rates, and effective integrals for a particular isotope are based on the flux existing in the presence of all the isotopes and, thus, may differ slightly from the results obtained from a pure sample of that isotope with the same surface to mass ratio.

The values printed out for each energy group are the group number, the upper and lower energy bounds, the total number of neutrons with an initial energy in that group, the total number with that group energy which enter the absorber region, the reaction rate per total neutron and per neutron entering the absorber and the effective resonance integral to that energy cutoff. This latter quantity is the I_{eff} between the upper energy limit and any given group cutoff energy.

The reaction rates described in the preceding paragraph may be used to determine the effective cadmium cutoff energy. The procedure is to run two cases, identical but for the presence of cadmium in one. Then, the cutoff energy is that energy in the non-cadmium case at which the reaction rate per entrant neutron is equal to the total reaction rate per entrant neutron in the cadmium covered case.

Finally, the sample mean (the effective resonance integral), variance, and probable error are printed out. These are based on the individual neutron results and the standard equations (ref. 17):

$$I_{eff} = \sum_{i=1}^{N} \frac{I_{eff}^{i}}{N} \tag{B4}$$

$$VAR = \sum \frac{\left(I_{eff}^{i}\right)^2}{N} - \left(I_{eff}\right)^2 \tag{B5}$$

$$\delta(I_{eff}) = P.E. = 0.6745 \sqrt{\frac{VAR}{N - 1}} \tag{B6}$$

Although standard methods may be used in the error analysis for directly sampled quantities such as the effective resonance integral, the use of the restart procedure in determining difference quantities, such as the Doppler coefficient, complicates the error analysis. Although alternate methods are possible, the method used in this report has been to set an upper limit to the probable error for restart cases by defining

$$P.E.(\alpha) = 0.6745 \sqrt{\frac{VAR_1 - VAR_2}{N - 1}} \tag{B7}$$

APPENDIX C

AUXILIARY PROGRAMS

The auxiliary programs used in selecting an energy - cross-section lattice, generating cross sections, and Doppler broadening the cross sections when temperature-dependent results are required are described. While any cross-section set with sufficient detail may be used in the Monte Carlo code, these programs make few approximations and should increase the accuracy of the calculation. There are three auxiliary programs.

EPIGRAM chooses an energy lattice spaced so that no more than a specified error is involved in interpolating the cross section between the lattice points chosen. The error specified may be an absolute difference in barns (cm^2) or a percent error in the absorption or total cross section.

BWSL generates cross sections by using the single level Breit-Wigner equation. To avoid the incorrect treatment (ref. 18) of interference between resonance and potential scattering, the equation is coded in complex number form.

DBCS Doppler broadens the cross sections obtained from BWSL. As the EPIGRAM code returns an energy lattice in which little error is incurred by interpolating between cross-section points, the DBCS code uses interpolated cross sections for numerical integration rather than require an evaluation of the single level Breit-Wigner equation at each point.

A brief resume of the equations, input and output, and comments on each of these programs, with the exception of EPIGRAM which is referenced elsewhere, follows.

BWSL

The cross sections used in the main program are generated by using the single level Breit-Wigner equations. The complex number forms of the equations were coded to avoid the occurrence of negative scattering cross sections which result from an incorrect treatment of the resonance and potential scattering interference. The equations for the scattering and absorption cross section are

$$\sigma_s(E) = 4\pi B\left(\frac{A+1}{A}\right)^2\left[\sum_k g_k\left|\sum_J\left(\frac{\lambda\!\!\!^{-}_{o,J}\frac{\Gamma_{n,J}}{2}}{E - E_{o,J} + i\frac{\Gamma_J}{2}}\right) - \lambda\!\!\!^{-}e^{-i\delta}\sin\delta\right|^2\right] \quad \text{(C1)}$$

$$\sigma_c(E) = \pi B\left(\frac{A+1}{A}\right)^2\sum_k g_k\lambda\!\!\!^{-}\sum_J\frac{\lambda\!\!\!^{-}_{o,J}\Gamma_n\Gamma_c}{\left(E - E_{o,J}\right)^2 + \left(\frac{\Gamma}{2}\right)^2} \quad \text{(C2)}$$

Equation (C2) is also used for fission cross sections when Γ_c is replaced by Γ_f. The symbols used denote

A target mass/neutron mass

B isotopic abundance

c capture

E incident neutron energy

f fission

g statistical weight factor

J summation over all resonances in an isotope having same g_k

k summation over all statistical weight factors

o value at resonance

R nuclear radius of target isotope

s scatter

δ phase shift, taken to be $-R/\lambda\!\!\!^{-}$

Γ nuclear level width

$\lambda\!\!\!^{-}$ rationalized wavelength

σ microscopic cross section

The scattering cross-section equation (eq. (C1)), due to summing the resonance part over all statistical weight factors with an attendant error in the potential scattering contribution, cannot be used directly. In the program, the potential scattering multiplied by

the statistical weight factor is subtracted from the expression given leaving the resonance and interference parts. When the summations are completed, the total potential scattering for that isotope is then added.

Input

NOGS	number of different g factors in each isotope
AA	atomic mass of each isotope
ABB	abundance of each isotope
RR	nuclear radius of each isotope
IEND	number of isotopes
LEND	number of energy points
E	energies
G1	g value of set of resonances
JEND	number of resonances with this g value
ERI	resonance energies
GAMG1	radiation widths
GAMN1	neutron widths
GAMF1	fission widths

DBCS

The Doppler broadening of the cross sections generated by BWSL is accomplished by this program. Rather than generate cross sections with the BWSL code at each point required in the numerical integration (eq. (C3)), the zero degree cross sections are interpolated, and a Simpson's rule integration with up to 400 points is performed. The equation used assumes a Maxwellian distribution for the target nuclei, and the integration is over all energies within which the exponential term e^{-x} lies within the limits $-88 \leq x \leq 88$

$$\sigma(E_n) = \int K \frac{1}{E_n} \sqrt{\frac{E}{T}}\, \sigma(E) \left\{ \exp\left[-\frac{A}{kT} \left(\sqrt{E_n} - \sqrt{E} \right)^2 \right] - \exp\left[-\frac{A}{kT} \left(\sqrt{E_n} + \sqrt{E} \right)^2 \right] \right\} dE \qquad \text{(C3)}$$

where k is the Boltzmann constant, T is the temperature in ^{o}K, E_n is the neutron energy at which the temperature dependent cross section is to be found, K is a constant, and the remaining symbols are the same as those defined for the BWSL code.

In order to obtain an accurate value for the infinitely dilute integral, the cross sections are assumed to vary linearly between energy points and the 1/E flux weighted resonance absorption integral

$$I = \int_{E_n}^{E_{n+1}} \left[\left(\frac{\sigma_{n+1} - \sigma_n}{E_{n+1} - E_n} \right) (E - E_n) + \sigma_n \right] \frac{dE}{E} \qquad \text{(C4)}$$

is printed out at each energy interval.

Input

A	atomic weight
T	temperature, ^{o}K
TEND	machine time to termination of run and final edit
NLEV	number of energy levels
ITYPES	flag for number of types of cross sections to be broadened; -1, 0, 1 for 1, 2, or 3 types
NPUNCH	if set equal to 1, the broadened cross sections are punched on cards
NEDU	upper energy at which broadening is performed
NEDL	lower energy at which the broadening is performed

As the integration relies on existing cross sections over an input energy range from NEDU to NEDL, the first and last few points may be in error. If this occurs, an error return states the fact and gives the energy cutoff actually used.

INTER	number of energies processed between time checks
E	energies in descending order
SIGC	capture cross sections
SIGS	scattering cross sections
SIGF	fission cross sections

The output consists of the energies with the corresponding broadened cross sections and resonance absorption integrals.

APPENDIX D

PROGRAM LISTINGS

Monte Carlo Program ERIDE

```
$IBJOB
$IBFTC ERI      LIST
      DIMENSION E(5000),S(5000),T(5000),SI(8),TI(8),RCYL(3),H(3),D(8),
     1A(8),N(8),KKK(8),ARATE(5),RHO(5),SMR(5),RRIN(5),ERI(5),NABS(8),
     2EG(100),EDR(100),SEDR(100),ERIP(100),NEST(100),NHST(100),DELU(100)
     3,GDIST(100),LLRN(7500)
      COMMON E,S,T
      COMMON/RDEP/LRN
      REWIND 1
      READ(5,501) EH,EL,XCAP,YCAP,ZCAP
  501 FORMAT(1P5E12.5)
      WRITE(6,500)XCAP,YCAP,ZCAP
  500 FORMAT(1H1/////10X,69HTHE OUTER MODERATOR DIMENSIONS, AT WHICH THE
     1 NEUTRON FLUX IS 1/E, ARE///14X,10HX BOUNDARY,10X,10HY BOUNDARY,10
     2X,10HZ BOUNDARY///5X,1P3E20.5)
      WRITE(6,508)EH,EL
  508 FORMAT(1HL,10X,38HTHE ENERGY RANGE FOR THIS CASE IS FROM,1PE12.5,2
     1X,2HTO,1PE12.5,2X,15HELECTRON VOLTS.)
      READ(5,505)NHIST,MIST,NREG,NISO,IGRP,INTER,NG,PHIBAS,TEND
  505 FORMAT(7I6,1P2E12.5)
      WRITE(6,506) NHIST,NREG,NISO,IGRP,INTER,PHIBAS,TEND
  506 FORMAT(1HL,10X,48HTHE INPUT DATA USED FOR THIS CASE IS AS FOLLOWS.
     1///116H     HISTORIES         NUMBER OF         NUMBER OF       ENERGI
     2ES  IN          TIME          FLUX IN ABSENCE      ESTIMATED/118H
     3REQUESTED          REGIONS          ABSORBERS       MAJOR  GROUP
     4  INTERVAL          OF ABSORBER       RUNNING TIME//I11,2I16,I17,I17
     5,1PE24.5,1PE18.5)
      NUTS=NREG-1
      NTOT=NISO+NUTS
      NEG=NG+1
      READ (5,502) (RCYL(I),H(I),I=1,NUTS)
  502 FORMAT(1P6E12.5)
      WRITE(6,503) (I,RCYL(I),H(I),I=1,NUTS)
  503 FORMAT(1HL,10X,49HTHE DIMENSIONS OF INNER CYLINDRICAL REGION NUMBE
     1R,I3,2X,3HARE,///20X,6HRADIUS,1PE13.5,2X,11HHALF HEIGHT,1PE13.5)
      READ (5,504) (N(I),D(I),A(I),I=1,NTOT)
  504 FORMAT(I12,1P2E12.5)
      WRITE(6,507) NISO,NTOT,(I,N(I),D(I),A(I),I=1,NTOT)
  507 FORMAT(1HL,10X,9HTHERE ARE,I3,2X,46HISOTOPES IN THE ABSORBER REGIO
     1N AND A TOTAL OF,I3,2X,10HMATERIALS.///62H     MATERIAL        FINAL
     2 ENERGY         NUCLEAR           ATOMIC/62H      NUMBER       LATTIC
     3E NUMBER        DENSITY           WEIGHT//(I9,I20,1PE19.5,1PE17.5))
      READ(5,509) (EG(J),J=1,NEG)
  509 FORMAT(1P6E12.5)
      M1=1
      DO 5000 J=1,NTOT
      NN=N(J)
      CALL BCREAD (E(M1),E(NN))
      CALL BCREAD (S(M1),S(NN))
      CALL BCREAD (T(M1),T(NN))
      M1=NN+1
 5000 CONTINUE
      READ(5,512) MATCH,LRN,NPCH,KSLB
  512 FORMAT(I3,O12,2I3)
 5050 CALL TIME1(TST)
      TSTART=TST/3600.0
      CN=ALOG(EH/EL)
      NMOD=0
      NESP=0
      NTAB=0
```

```
      KENT=0
      NENT=0
      NEECL=0
      ADIST=0.0
      NAB1=0
      NAB2=0
      NAB3=0
      NAB4=0
      NAB5=0
      XX=0.0
      XS=0.0
      MISTY = MIST
      DO 5001 J=1,NG
      NEST (J) = 0
      NHST(J) = 0
      GDIST(J)=0.0
      EDR(J)=0.0
 5001 SEDR(J)=0.0
      DO 5003 L=1,NISO
 5003 ARATE(L)=0.0
      BDIST=0.0
      CDIST=0.0
      DDIST=0.0
      RDIST=0.0
      NOUT=(NHIST/MIST)+1
      NREM=NHIST-MIST*(NOUT-1)
      JINTER=INTER+MIST
      DO 1003 IO=1,NOUT
      JINTER=JINTER-MIST
      LAT=0
      IF(NOUT.EQ.IO)GO TO 1007
      IF(MATCH.EQ.0) GO TO 1005
      READ(1) MIST,(LLRN(LAT),LAT=1,MIST)
      GO TO 1005
 1007 MIST=NREM
      IF(NREM.LE.0) GO TO 1003
      IF(MATCH.EQ.0) GO TO 1005
      READ(1) MIST,(LLRN(LAT),LAT=1,MIST)
 1005 DO 1000 I=1,MIST
      IF(I.LT.JINTER)GO TO 1111
      JINTER=JINTER+INTER
      CALL TIME1(TST)
      TPRES=TST/3600.0
      TIME=TPRES-TSTART
      IF(TIME.LT.TEND)GO TO 1111
      NHIST = (IO-1)*MISTY+I-1
      IF(NPCH.EQ.0) GO TO 1101
      KENT=NENT-KENT
      WRITE(1) KENT,(LLRN(LAT),LAT=1,KENT)
      GO TO 1101
 1111 CONTINUE
      KKK(1)=1
      NK=NTOT-1
      DO 2101 J=1,NK
 2101 KKK(J+1)=N(J)+1
      INSAP=0
      K=0
      M=NREG
      INRUP=1
      XV=0.0
```

```
520 IF(K-1)525,535,535
525 IF(MATCH.EQ.0)GO TO 530
    LAT=LAT+1
    LRN=LLRN(LAT)
530 CALL INIPOS(XCAP,YCAP,ZCAP,XO,YO,ZO,IN,IGN,KLRN)
    ELA=ESTART(EL,EH,CN)
    DO 536 IHST=1,NG
    IF(ELA.LT.EG(IHST).AND.ELA.GE.EG(IHST+1))GO TO 537
536 CONTINUE
537 NHST(IHST)=NHST(IHST)+1
535 CALL ISOTRO(WX,WY,WZ,K,IN,IGN)
    IF(K-1)550,540,540
540 CALL CMLAB(WX,WY,WZ,ELA,A(II),CX,CY,CZ)
    IF(ELA-EL)545,545,551
545 INRUP=2
    GO TO (551,950,551,551),INRUP
550 K=1
551 CONTINUE
    CX=WX
    CY=WY
    CZ=WZ
552 CONTINUE
    IF(M.GT.1)GO TO 710
    NS=1
    SIGT=0.0
    SIGA=0.0
610 DO 650 L=1,NISO
    NF=N(L)
    IF(KKK(L).GT.NS)GO TO 616
    DO 612 K=NS,NF,IGRP
    KK=K
    IF(E(K)-ELA)614,614,612
612 CONTINUE
    KK=NS+IGRP
614 K=KK-IGRP
    GO TO 618
616 K=KKK(L)
618 DO 620 K=K,NF
    KK=K
    IF(E(K)-ELA)630,620,620
620 CONTINUE
630 K=KK-1
    AM=(S(K)-S(K+1))/(E(K)-E(K+1))
    BS=S(K)-AM*E(K)
    SI(L)=AM*ELA+BS
    TM=(T(K)-T(K+1))/(E(K)-E(K+1))
    BT=T(K)-TM*E(K)
    TI(L)=TM*ELA+BT
    SIGT=SIGT+D(L)*TI(L)
    SIGA=SIGA+D(L)*(TI(L)-SI(L))
    NS=NF+1
    KKK(L)=K
650 CONTINUE
    CALL ISOPIK(NISO,II,D,TI,SIGT)
    GO TO 553
710 L=NISO+M-1
    II=L
    NS=N(L-1)+1
    NF=N(L)
    IF(KKK(L).GT.NS)GO TO 716
```

```
      DO 712 K=NS,NF,IGRP
      KK=K
      IF(E(K)-ELA)714,714,712
  712 CONTINUE
      KK=NS+IGRP
  714 K=KK-IGRP
      GO TO 718
  716 K=KKK(L)
  718 DO 720 K=K,NF
      KK=K
      IF(E(K)-ELA)730,720,720
  720 CONTINUE
  730 K=KK-1
      L=NISO+M-1
      XM=(S(K)-S(K+1))/(E(K)-E(K+1))
      BX=S(K)-XM*E(K)
      SI(L)=XM*ELA+BX
      XMT=(T(K)-T(K+1))/(E(K)-E(K+1))
      BXT=T(K)-XMT*E(K)
      TI(L)=XMT*ELA+BXT
      KKK(L)=K
  553 CONTINUE
      CALL MFP (TI(II),DIST,D(II))
      MM=M
      NFLG = 1
      ISET=0
  555 IF(MM-NREG)1510,1521,2000
 1510 CALL CYLTCK(-1,IFLG,RCYL(MM ),H(MM ),DIST,XO,YO,ZO,WX,WY,WZ)
      IF(IFLG.EQ.-1) HZ=H(MM)
      ISET=IFLG
      NFLG=IABS(IFLG)+1
      M=M+IABS(IFLG)
 1520 IF(MM-1)2000,1516,1521
 1521 CALL CYLTCK(+1,IFLG,RCYL(MM-1),H(MM-1),DIST,XO,YO,ZO,WX,WY,WZ)
      IF(IFLG.EQ.-1) HZ=H(MM-1)
      ISET=ISET+2*IFLG
      M=M-NFLG*IABS(IFLG)
 1516 IF((MM-1).NE.0.OR.INSAP.NE.0)GO TO 5556
      INSAP=1
      DO 5557 IEST=1,NG
      IF(ELA.LT.EG(IEST).AND.ELA.GE.EG(IEST+1))GO TO 5559
 5557 CONTINUE
 5559 NEST(IEST)=NEST(IEST)+1
      IF(MATCH.NE.0)GO TO 5556
      LAT=LAT+1
      LLRN(LAT)=KLRN
 5556 CALL XOYOZO(DIST,WX,WY,WZ,XCAP,YCAP,ZCAP,XO,YO,ZO,HZ,ISET,INRUP)
      GO TO (5550,5552,5553,5554),MM
 5550 CONTINUE
      IF(KSLB.EQ.0)GO TO 5549
      DIST=DIST*ABS(WZ)
 5549 ADIST=ADIST+DIST
      XIND=DIST*SIGA
      XX=XX+XIND
      XV=XV+XIND
      DO 5551 L=1,NISO
      ARATE(L)=ARATE(L)+DIST*D(L)*(TI(L)-SI(L))
 5551 CONTINUE
      DO 5560 IEG=1,NG
      IF(ELA.LT.EG(IEG).AND.ELA.GE.EG(IEG+1))GO TO 5565
```

```
5560 CONTINUE
5565 EDR(IEG)=EDR(IEG)+DIST*SIGA
     GDIST(IEG)=GDIST(IEG)+DIST
     GO TO 5558
5552 BDIST=BDIST+DIST
     GO TO 5558
5553 CDIST=CDIST+DIST
     GO TO 5558
5554 DDIST=DDIST+DIST
5558 RDIST=RDIST+DIST
     GO TO (560,560,960,560),INRUP
 560 IF(MM-M)552,572,552
 572 CONTINUE
     CALL INTACT(SI(II),TI(II),INRUP)
     GO TO (535,535,535,970),INRUP
 950 NMOD=NMOD+1
     NENT=NENT+INSAP
     GO TO 999
 960 NESP=NESP+1
     IF(INSAP.EQ.0)GO TO 965
     NEECL=NEECL+1
 965 NENT=NENT+INSAP
     GO TO 999
 970 IF(M-1)980,974,980
 974 GO TO (975,976,977,978,979),II
 975 NAB1=NAB1+1
     GO TO 980
 976 NAB2=NAB2+1
     GO TO 980
 977 NAB3=NAB3+1
     GO TO 980
 978 NAB4=NAB4+1
     GO TO 980
 979 NAB5=NAB5+1
 980 NTAB=NTAB+1
     NENT=NENT+INSAP
 999 XS=XS+XV*XV
1000 CONTINUE
     IF(NPCH.EQ.0) GO TO 1003
     KENT=NENT-KENT
     WRITE(1) KENT,(LLRN(LAT),LAT=1,KENT)
     KENT=NENT
1003 CONTINUE
1101 WRITE(6,1124)
1124 FORMAT(1H1)
     IF(KSLB.NE.0)GO TO 1130
     WRITE(6,1126)
1126 FORMAT(1HL,10X,46HTHIS CASE IS FOR A THREE DIMENSIONAL CYLINDER.)
     GO TO 1001
1130 WRITE(6,1128)
1128 FORMAT(1HL,10X,34HTHIS CASE IS FOR AN INFINITE SLAB.)
1001 WRITE(6,1100)NHIST,NENT,NEECL,NAB1,NAB2,NAB3,NAB4,NAB5,NTAB,NMOD,N
    1ESP
1100 FORMAT(1HL,10X,37HRESULTS FOR THIS CASE ARE AS FOLLOWS.////119H HI
    1STORIES   ENTERING   ESCAPING          NEUTRONS ABSORBED BY ISOTO
    2PE NUMBER             TOTAL    MODERATED   ESCAPED/98H    RUN
    3 CYLINDER   CYLINDER     ONE         TWO        THREE       FOUR
    4   FIVE     ABSORBED//I8,2I11,I10,2I11,I10,I12,I13,I10,I12)
     H=ABS(H)
     PHIT=CN
```

```
      VSAM=6.2832*RCYL*RCYL*H
      SURC=6.2832*RCYL*(RCYL+2.0*H)
      IF(KSLB.EQ.0)GO TO 1120
      VSAM=H
      SURC=1.0
 1120 FN=FLOAT(NENT)
      FH=FLOAT(NHIST)
      DT=0.0
      ARTOT=0.0
      DO 1150 L=1,NISO
      RHO(L)=D(L)*A(L)/0.6025
      DT=DT+D(L)
      SMR(L)=SQRT(SURC/(RHO(L)*VSAM))
      RRIN(L)=ARATE(L)/FLOAT(NENT)
      ERI(L)=(RRIN(L)*PHIT)/(D(L)*PHIBAS)
      RHOT=RHOT+RHO(L)
      ARTOT=ARTOT+ARATE(L)
 1150 CONTINUE
      WRITE(6,1250) (L,RHO(L),SMR(L),RRIN(L),ERI(L),L=1,NISO)
 1250 FORMAT(1HL,99H      ABSORBER              DENSITY            SQUARE R
     1OOT      REACTION RATE PER   EFFECTIVE RESONANCE/12H      NUMBER,34
     2X,48HOF  S/M          INCIDENT NEUTRON         INTEGRAL//I10,6X,1P4E
     320.5)
      SUME=0.0
      SDELU=0.0
      FNEST=0.0
      FNHST=0.0
      DO 1160 IG=1,NG
      FNEST=FNEST+FLOAT(NEST(IG))
      FNHST=FNHST+FLOAT(NHST(IG))
      DELU(IG)=ALOG(EG(IG)/EG(IG+1))
      SDELU=SDELU+DELU(IG)
      SUME=SUME+EDR(IG)
      IF(GDIST(IG).EQ.0.0) GO TO 1158
      GDIST(IG)=EDR(IG)/GDIST(IG)
 1158 SEDR(IG)=SUME/FNHST
      EDR(IG)=SUME/FNEST
 1160 ERIP(IG)=SUME*SDELU/(DT*PHIBAS*FNEST)
      WRITE(6,1105)
 1105 FORMAT(1HL,10X,93HTHE REACTION RATE IN THE ABSORBER, PER TOTAL ENT
     1RANT NEUTRON, BY ENERGY GROUP, IS AS FOLLOWS.)
      WRITE(6,1106) (IG,EG(IG),EG(IG+1),NHST(IG),NEST(IG),SEDR(IG),EDR(I
     2G),ERIP(IG),IG=1,NG)
 1106 FORMAT(1HL,112H   GROUP        UPPER              LOWER      NSTART
     2  NENTER     NORMALIZED RATE TO LOWER LIMIT     TOTAL IEFF TO/111H
     3  NUMBER       ENERGY            ENERGY          IN GROUP         P
     4ER TOTAL N     PER ENTRANT N      LOWER LIMIT//(I6,1P2E18.5,2I8,1P
     53E18.5))
      ADIST = ADIST/FLOAT(NENT)
      SMRT=SQRT(SURC/(RHOT*VSAM))
      RTIN=ARTOT/FLOAT(NENT)
      ERIT=(RTIN*PHIT)/(DT*PHIBAS)
      WRITE(6,1107) ADIST
1107  FORMAT (1HL,65HTHE INTEGRATED FLUX PER ENTRANT NEUTRON IN THE ABSO
     $RBER REGION IS,1PE15.5)
      WRITE(6,1200) PHIT,SURC,VSAM,RHOT,SMRT,RTIN,ERIT
 1200 FORMAT(1HL,10X,20HTOTALS FOR THE CASE.///115H   LETHARGY       ABS
     1ORBER       ABSORBER         DENSITY      SQUARE ROOT   REACTION RA
     2TE PER   EFFECTIVE RESONANCE/40H   INTERVAL       SURFACE
     3VOLUME,24X,45HOF  S/M       INCIDENT NEUTRON        INTEGRAL//1PE13
```

```
     4.5,1P2E15.5,1P2E15.5,1PE17.5,1PE22.5)
      FN=FLOAT(NENT)
      DEN=PHIT/(DT*PHIBAS)
      XX=XX*DEN/FN
      XS=(XS*DEN*DEN/FN)-(XX*XX)
      DELX=0.6745*SQRT(XS/(FN-1.0))
      WRITE(6,1213) XX,XS,DELX
 1213 FORMAT(1HL,42H     SAMPLE          VARIANCE          PROBABLE/10H
     1MEAN,26X,5HERROR//1PE14.5,1PE15.5,1PE16.5)
      IF(MATCH.NE.0)GO TO 1298
      IF(NPCH.EQ.0) GO TO 1299
      WRITE(6,1275)NENT
 1275 FORMAT(1HL,10X,46HOCTAL CARDS HAVE BEEN PUNCHED WHICH WILL FORCE,I
     16,2X,38HNEUTRONS TO ENTER THE ABSORBER REGION.)
      WRITE(6,1277) IO
 1277 FORMAT(1HL,10X,38HTHE NUMBER OF OUTER LOOPS COMPLETED IS,I4,1H.)
      GO TO 1299
 1298 WRITE(6,1274)NENT
 1274 FORMAT(1HL,10X,23HTHIS CASE WAS RUN USING,I6,2X,77HOCTAL RESTART N
     1UMBERS WHICH FORCED EACH NEUTRON TO ENTER THE ABSORBER REGION.)
 1299 CONTINUE
      WRITE(6,2020) LRN
 2020 FORMAT(1HL,10X,57HTHE LAST RANDOM NUMBER COEFFICIENT USED IN THIS
     1SERIES IS,3X,O12)
      WRITE(6,9999) (GDIST(IG),IG=1,NG)
 9999 FORMAT(1HL,1P6E12.5)
      REWIND 1
      CALL EXIT
 2000 WRITE(6,2001)
 2001 FORMAT(20H TROUBLE IN INDICES.)
      STOP
      END
$IBFTC GEN      LIST
      SUBROUTINE RANDM(R,F)
      COMMON/RDEP/LRN
      LRN=LRN*30517578125
      ZR=2.91038304567E-11
      R=FLOAT(LRN)*ZR
      RETURN
      END
$IBFTC PROSIT   LIST
      SUBROUTINE INIPOS(XCAP,YCAP,ZCAP,XO,YO,ZO,IN,IGN,KLRN)
      COMMON/RDEP/LRN
      IGN=1
      AX=YCAP*ZCAP
      AY=XCAP*ZCAP
      AZ=XCAP*YCAP
      AT=AX+AY+AZ
      RX=AX/AT
      RY=AY/AT
      KLRN=LRN
      CALL RANDM(R1,1)
      XO=XCAP*(1.0-2.0*R1)
      CALL RANDM(R2,1)
      YO=YCAP*(1.0-2.0*R2)
      CALL RANDM(R3,1)
      ZO=ZCAP*(1.0-2.0*R3)
  300 CALL RANDM(R4,1)
      IF(R4-RX-RY)310,320,320
  310 IF(R4-RX)340,330,330
```

```
  320 Z0=ZCAP*(Z0/ABS(Z0))
      IN=1
      IF(Z0.GT.0.0)GO TO 350
      IGN=-1
      GO TO 350
  330 Y0=YCAP*(Y0/ABS(Y0))
      IN=0
      IF(Y0.GT.0.0)GO TO 350
      IGN=-1
      GO TO 350
  340 X0=XCAP*(X0/ABS(X0))
      IN=-1
      IF(X0.GT.0.0)GO TO 350
      IGN=-1
  350 CONTINUE
      RETURN
      END
$IBFTC EOPEN   LIST
      FUNCTION ESTART (EL,E1,CN)
      COMMON/RDEP/LRN
      CALL RANDM(R30,1)
      ESTART=EL*EXP(R30*CN)
      RETURN
      END
$IBFTC CORIEN  LIST
      SUBROUTINE ISOTRO(WX,WY,WZ,K,IN,IGN)
      COMMON/RDEP/LRN
  100 CALL RANDM(R7,1)
      WZ=R7+R7-1.0
      SNT=SQRT(1.0-WZ*WZ)
  120 CALL RANDM(R8,1)
      CALL RANDM(R9,1)
      D=R9+R9-1.0
      E=R8*R8
      F=E+D*D
      IF(F-1.0)130,130,120
  130 WX=SNT*(E+E-F)/F
      WY=SNT*(2.0*R8*D)/F
      T=WX*WX+WY*WY+WZ*WZ
      T=SQRT(T)
      WX=WX/T
      WY=WY/T
      WZ=WZ/T
      IF(K-1)135,190,190
  135 IF(IN)140,150,160
  140 IF(IGN.GT.0)GO TO 142
      IF(WX)100,190,190
  142 IF(WX)190,190,100
  150 IF(IGN.GT.0)GO TO 152
      IF(WY)100,190,190
  152 IF(WY)190,190,100
  160 IF(IGN.GT.0)GO TO 162
      IF(WZ)100,190,190
  162 IF(WZ)190,190,100
  190 CONTINUE
      RETURN
      END
$IBFTC LUTATE  LIST
      SUBROUTINE CMLAB(WX,WY,WZ,ELA,A,CX,CY,CZ)
      COMMON/RDEP/LRN
```

```
      ELB=ELA
      Z=A/1.00898
  230 CMU=CX*WX+CY*WY+CZ*WZ
      CKON=SQRT(1.0+Z*Z+2.0*Z*CMU)
      WX=(CX+Z*WX)/CKON
      WY=(CY+Z*WY)/CKON
      WZ=(CZ+Z*WZ)/CKON
      ELA=(ELB*CKON*CKON)/((Z+1.0)*(Z+1.0))
      CONTINUE
      RETURN
      END
$IBFTC FLIGHT  LIST
      SUBROUTINE MFP(SIGT,DIST,D)
      COMMON/RDEP/LRN
      CALL RANDM(R10,1)
      FNMFP=-ALOG(R10)
      SIGMAC=D*SIGT
 2020 DIST=FNMFP/SIGMAC
      RETURN
      END
$IBFTC GOK     LIST
      SUBROUTINE CYLTCK(N,IFLG,RCYL,H,SM,XO,YO,ZO,WX,WY,WZ)
      COMMON/RDEP/LRN
      SQRTF(X)=SQRT(X)
      QUADRA(Q)=A*Q**2+2.0*B*Q+C
      IFLG=0
      H=ABS(H)
      EPSI=1.0E-4
      IF(N)2,97,3
    2 A=1.0-WZ**2
      B=XO*WX+YO*WY
      C=XO**2+YO**2-(RCYL*RCYL)
      IF(WZ)4,5,6
    4 H=-H
    6 T=(-ZO+H)/WZ
      IF(T)97,8,9
    8 IFLG=-1
      GO TO 40
    9 IF(QUADRA(T))10,10,5
    5 IF(QUADRA(SM))99,99,11
   11 E=B**2-A*C
      IF(E)12,13,14
   14 SM=(-B+SQRTF(E))/A
      IFLG=1
      GO TO 99
   10 IF(T-SM)15,99,99
   15 SM=T
      IFLG=-1
      GO TO 99
    3 IF(ZO+H)16,16,17
   17 IF(ZO-H)18,19,19
   19 IF(WZ)220,99,99
   16 IF(WZ)99,99,20
  220 H=-H
   20 C=XO**2+YO**2-(RCYL*RCYL)
      B=XO*WX+YO*WY
      IF(C)21,22,22
   22 IF(B)23,99,99
   21 A=1.0-WZ**2
      U=-(ZO+H)/WZ
```

```
      IF(QUADRA(U))24,99,99
   23 A=1.0-WZ**2
      E=B**2-A*C
      IF(E)99,99,25
   25 U=-(Z0+H)/WZ
      IF(QUADRA(U))24,24,26
   26 IF(A*U+B)27,99,99
   24 IF(U-SM)28,99,99
   28 SM=U
      H=-H
      IFLG=-1
      GO TO 99
   18 C=X0**2+Y0**2-(RCYL*RCYL)
      B=X0*WX+Y0*WY
      IF(C)29,30,30
   30 IF(B)31,99,99
   31 A=1.0-WZ**2
      E=B**2-A*C
      IF(E)99,99,32
   32 IF(WZ)33,34,27
   33 H=-H
   27 T=(-Z0+H)/WZ
      IF(A*T+B)35,34,34
   35 IF(QUADRA(T))34,99,99
   34 IF(A*SM+B)36,37,37
   37 SM=-(B+SQRTF(E))/A
      IFLG=1
      GO TO 99
   36 IF(QUADRA(SM))37,99,99
   29 IF(B)229,99,99
  229 IF(-C-EPSI)13,13,97
   12 IF(-E-EPSI)13,13,97
   13 IFLG=1
   40 SM=0.0
      GO TO 99
   99 CONTINUE
   50 CONTINUE
   51 CONTINUE
      RETURN
   97 WRITE(6,98)
   98 FORMAT(20H      CYLINDER SNAFU.)
      GO TO 51
      END
$IBFTC UPDIST  LIST
      SUBROUTINE XOYOZO(DIST,WX,WY,WZ,XCAP,YCAP,ZCAP,X0,Y0,Z0,HZ,ISET,IN
     1RUP)
      COMMON/RDEP/LRN
      X00=X0+WX*DIST
      XTEST=ABS(X00)-XCAP
      IF(XTEST)910,910,915
  915 DIST=(ABS(X00-X0)-XTEST)/ABS(WX)
      INRUP=3
  910 Y00=Y0+WY*DIST
      YTEST=ABS(Y00)-YCAP
      IF(YTEST)920,920,925
  925 DIST=(ABS(Y00-Y0)-YTEST)/ABS(WY)
      INRUP=3
  920 Z00=Z0+WZ*DIST
      ZTEST=ABS(Z00)-ZCAP
      IF(ZTEST)930,930,935
```

```
  935 DIST=(ABS(ZOO-ZO)-ZTEST)/ABS(WZ)
      INRUP=3
  930 CONTINUE
      GO TO (940,940,950),INRUP
  940 XO=XOO
      YO=YOO
      ZO=ZOO
      IF(ISET.LT.0) ZO=HZ
  950 RETURN
      END
$IBFTC ZAP      LIST
      SUBROUTINE INTACT(SIGS,SIGT,INRUP)
      COMMON/RDEP/LRN
      CALL RANDM(R11,1)
      IF(R11-(SIGS/SIGT))810,810,830
  830 INRUP=4
  810 CONTINUE
      RETURN
      END
$IBFTC WHABS    LIST
      SUBROUTINE ISOPIK (NISO,II,D,TI,SIGT)
      COMMON D(8),TI(8)
      COMMON/RDEP/LRN
      TCS=0.0
      CALL RANDM(R41,1)
      DO 4003 NIS=1,NISO
      TCS=TCS+D(NIS)*TI(NIS)
      IF(R41-(TCS/SIGT))4005,4005,4003
 4003 CONTINUE
 4005 II=NIS
      RETURN
      END
```

Single Level Breit-Wigner Program BWSL

```
$IBJOB
$IBFTC SECTBS
      DIMENSION ER( 500),GAMN( 500),GAMG( 500),GAMF( 500),GAMNO( 500)
      DIMENSION G(100),ER1(100),GAMN1(100),GAMG1(100),GAMF1(100),JENDA
     $(100)
      DIMENSION E(2000),SIGS(2000),SIGC(2000),SIGF(2000),SIGP(2000),
     $SIGT(2000),TEMPA(2000),TEMPB(2000)
      DIMENSION AA(10),ABB(10),RR(10),NOGS(10)
      DIMENSION  CSINT(10),FSINT(10),TOTSIN(10)
      COMPLEX DEN,EX1,T1,T2,CEXP1,SUMJT1,VAL3
      REAL LAM,LAMR
      DATA PI/3.1415926/,CONS/2.86E-9/
      NAMELIST /IN/ NOGS,AA,ABB,RR,IEND
      READ(5,IN)
      READ(5,101) LEND,(E(I),I=1,LEND)
101   FORMAT(I6/(1P6E12.5))
      SIGP(1) = 0.
      SIGS(1) = 0.
      SIGC(1) = 0.
      SIGF(1) = 0.
      SIGT(1) = 0.
      DO 102 I=1,IEND
      A = AA(I)
      AB = ABB(I)
      R = RR(I)
      NGS = NOGS(I)
      WRITE(6,10) IEND,I,AB,A,R
10    FORMAT(1H1,//////53X,I3,2X,8HISOTOPES////////30X,7HISOTOPE,10X,
     $9HABUNDANCE,10X,13HATOMIC WEIGHT,10X,12HNUCLEAR RAD./32X,I3,10X,
     $1PE14.7,7X,E14.7,8X,E14.7)
      FA = ((A+1.008986)/A)**2
      DO 100 L = 1,LEND
      NSUMG = 0
      GSUM = 0.
      CSUM = 0.
      FSUM = 0.
      LAM = CONS/SQRT(E(L))
      BLAM = LAM/PI/2.
      PSIG = FA*AB*PI*1.E24
      JS = 1
      JN = 0
      JE = 0
      JG = 0
      NJ = 0
      JENDA(NJ) = 0
      IF (L .GE. 2) GO TO12
      JR = 0
1000  READ(5,1) G1,JEND,(ER1(JJ),GAMG1(JJ),GAMN1(JJ),GAMF1(JJ),JJ=1,JEND
     $)
1     FORMAT (E12.0,I6/(4E12.8))
      JG = JG + 1
      G(JG) = G1
      JN = 1 + JN
      JENDA (JN) = JEND
      DO 8 J1 = 1,JEND
      JR = 1 + JR
      IF(J1 .EQ. 1) JRS = JR
      IF(J1 .EQ. JEND) JRE = JR
      ER(JR) = ER1(J1)
      GAMN(JR) = GAMN1(J1)
```

```
      GAMNO(JR) = 0.
      GAMG(JR) = GAMG1(J1)
8     GAMF(JR) = GAMF1(J1)
      WRITE (6,15)G1,JEND,(JJ,ER(JJ),GAMN(JJ),GAMNO(JJ),GAMG(JJ),GAMF(JJ
     $),JJ=JRS,JRE)
15    FORMAT(1HL,//////////46X,7HG VALUE,12X,17HTOTAL NO. OF RES./42X,1P
     $E14.7,15X,I3/////16X,8HRES. NO.,10X,8HENERGY 0,10X,7HGAMMA N,10X,
     $8HGAMMA NO,10X,7HGAMMA G,14X,7HGAMMA F/ (19X,I3,9X,1PE14.7,5X,
     $E14.7,4X,E14.7,5X,E14.7,5X,E14.7)     )
      GO TO 16
12    JG = JG + 1
      JN = JN + 1
16    SUMJT1 = (0.,0.)
      SUMCT1 = 0.
      SUMFT1 = 0.
      JS = JS + JENDA(JN-1)
      JE = JE + JENDA(JN)
      DO 20 J = JS,JE
      LAMR = CONS/SQRT(ABS(ER(J)))
      BLAMR = LAMR/PI/2.
      P1 = E(L) - ER(J)
      GAM = GAMN(J) + GAMG(J) + GAMF(J)
      P2 = GAM/2.
      DEN = CMPLX(P1,P2)
      CPF =BLAMR* GAMN(J)/(P1**2 + P2**2)
      T1 =(GAMN(J)/2./DEN)*BLAMR
      DEBUG LAMR,BLAMR,P1,GAM,DEN,T1
      CT1 = CPF*GAMG(J)
      FT1 = CPF *GAMF(J)
      SUMFT1 = FT1+SUMFT1
      SUMCT1 = CT1 + SUMCT1
20    SUMJT1 = T1 + SUMJT1
      DEL = -R/BLAM
      VAL2 = SIN(DEL)
      EX1 = CMPLX(0.,-DEL)
      CEXP1 = CEXP(EX1)
      T2 = CEXP1*VAL2*BLAM
      ABT2 = CABS(T2)
      VAL3 = SUMJT1-T2
      VAL1 = CABS(VAL3)
      SIGSP = VAL1**2 - ABT2**2
      DEBUG SUMJT1,DEL,VAL2,EX1,CEXP1
      DEBUG T2,ABT2,VAL3,VAL1,SIGSP
94    NSUMG = NSUMG + 1
      GPIECE = G(JG)*SIGSP
      GSUM = GPIECE + GSUM
      CPIECE = G(JG)*SUMCT1
      CSUM = CPIECE + CSUM
      FPIECE = G(JG)*SUMFT1
      DEBUG I,L,JG,G(JG),GPIECE,GSUM,NGS,NSUMG
      FSUM = FPIECE + FSUM
      IF (L .GE. 2) GO TO 98
      IF(NGS .NE. NSUMG) GO TO 1000
      GO TO 99
98    IF(NGS .NE. NSUMG) GO TO 12
99    SIG1 = 4.*PSIG*GSUM
      SIG2 = 4.*PSIG*ABT2**2
      SIGP(L) = SIG2+SIGP(L)
      SIGS(L) = SIG1+SIG2+SIGS(L)
      TEMPA(L) = PSIG*CSUM*BLAM
```

```
      SIGC(L) = TEMPA(L) + SIGC(L)
      TEMPB(L) = PSIG*FSUM*BLAM
      SIGF(L) = TEMPB(L) + SIGF(L)
      SIGF(L) = PSIG*FSUM*BLAM    + SIGF(L)
  100 SIGT(L) = SIGS(L)+SIGC(L)+SIGF(L)
      CALL ABSIN(E,TEMPA,TEMPB,LEND,CABSIN,FABSIN)
      CSINT(I) = CABSIN/AB
      FSINT(I) = FABSIN/AB
      TOTSIN(I) = CSINT(I) + FSINT(I)
102   CONTINUE
      WRITE(6,159)
  159 FORMAT(1H1)
      WRITE(6,160) (I,CSINT(I),FSINT(I),TOTSIN(I),I=1,IEND)
  160 FORMAT(1H3,27X,64HISOTOPE            CAPTURE            FISSION
     1       ABSORPTION/28X,62HNUMBER           INTEGRAL           INTEGRA
     2L            INTEGRAL///(I31,1PE24.5,1PE17.5,1PE19.5))
      WRITE(6,80)(LL,E(LL),SIGS(LL),SIGP(LL),SIGC(LL),SIGF(LL),SIGT(LL),
     $LL=1,LEND)
80    FORMAT(1H1////5X,6HLEVEL,12X,6HENERGY,12X,7HSIGMA S,12X,7HSIGMA P,
     $12X,7HSIGMA C,12X,7HSIGMA F,12X,7HSIGMA T/(5X,I3,10X,1PE14.7,5X,E1
     $4.7,5X,E14.7,5X,E14.7,5X,E14.7,5X,E14.7)  )
      WRITE(6,111) (E(I),SIGC(I),SIGS(I),SIGF(I),I=1,LEND)
111   FORMAT(1H$,1P4E12.5)
      STOP
      END
$IBFTC ABSIN1  LIST
      SUBROUTINE ABSIN (E,TEMPA,TEMPB,LEND,CABSIN,FABSIN)
      DIMENSION E(2000),TEMPA(2000),TEMPB(2000)
      CABSIN = 0.0
      FABSIN = 0.0
      DO 100 I=2,LEND
      XNAME = ALOG(E(I)/E(I-1))
      CABSIN = CABSIN +((TEMPA(I) + TEMPA(I-1))/2. )*XNAME
100   FABSIN = FABSIN +((TEMPB(I) + TEMPB(I-1))/2.)*XNAME
      RETURN
      END
$DATA
```

Doppler Broadening Program DBCS

```
$IBJOB
$IBFTC DBCS    LIST
       COMMON NLEV,I,J,Z,CON,DBI,E,SIGC,SIGS,SIGF,ITYPES,NEDU,NEDL
       COMMON EPSU,KSAV
       DIMENSION E(2200),SIGC(2200),SIGS(2200),SIGF(2200),SIGT(2200),
      $DBIC(2200),DBIS(2200),DBIF(2200)
       EXTERNAL DBO
 1000  READ(5,1010) A,T,TEND,NLEV,ITYPES,NPUNCH,NEDU,NEDL,INTER
 1010  FORMAT(1P3E12.5,6I6)
       READ(5,1020) (E(I),SIGS(I),SIGT(I),I=1,NLEV)
 1020  FORMAT(1P3E12.5)
       DO 10 JK=1,NLEV
   10  SIGC(JK)=SIGT(JK)-SIGS(JK)
       KSAV = 1
       JINTER = NEDU
       CALL TIME1(TS)
       Z=A/(8.6167E-5*T)
       CON=SQRT(A/(1.0828E-3*T))
       DO 2000 I=NEDU,NEDL
       I=I
       IF(I .NE. JINTER) GO TO 1050
       JINTER = JINTER + INTER
       CALL TIME1(TP)
       TELAP = (TP-TS)/3600.
       IF(TELAP .LT. TEND) GO TO 1050
       NEDL = JINTER-INTER-1
       GO TO 2010
1050   EPSL=((SQRT (E(I))-SQRT (88.0/Z))**2)
       EPSU=((SQRT (E(I))+SQRT (88.0/Z))**2)
       IF(EPSL-E(NLEV))1540,1550,1550
 1540  EPSL=E(NLEV)
       WRITE (6,3050) E(NLEV),I
 3050  FORMAT(1HL,10X,49HTHE LOWER INTEGRATION LIMIT HAS BEEN SET EQUAL T
      1O1PE12.5,12H FOR SET NO.I6)
 1550  CONTINUE
       IF(EPSU-E(1))1570,1570,1560
 1560  EPSU=E(1)
       WRITE(6,3075) E(1),I
 3075  FORMAT(1HL,10X,49HTHE UPPER INTEGRATION LIMIT HAS BEEN SET EQUAL T
      1O1PE12.5,12H FOR SET NO.I6)
 1570  CONTINUE
       NTYPES=ITYPES+2
       DO 1090 J=1,NTYPES
       J=J
       DBI=EXPS1 (EPSL,EPSU,DBO,KK)
       GO TO (1060,1070,1080),J
 1060  DBIC(I)=DBI
       GO TO 1090
 1070  DBIS(I)=DBI
       GO TO 1090
 1080  DBIF(I)=DBI
 1090  CONTINUE
       SIGT(I)=DBIC(I)+DBIS(I)+DBIF(I)
 2000  CONTINUE
2010   WRITE(6,3000) NEDL
3000   FORMAT(1H1//////40X,16HNO. OF ENERGYS =,I5      )
       WRITE(6,3005) A,T
 3005  FORMAT(1HL,5X,43HTHESE ARE CROSS-SECTIONS FOR ISOTOPE NUMBER1PE12.
      15/1H ,2X,20HDOPPLER BROADENED TO1PE12.5,16H DEGREES KELVIN.////1H
      2,3X,6HENERGY,9X,7HSIGMA C,8X,7HSIGMA S,8X,7HSIGMA F,8X,7HSIGMA T)
```

```
      WRITE(6,3010) (E(I),DBIC(I),DBIS(I),DB1F(I),SIGT(I),I=NEDU,NEDL)
 3010 FORMAT(1P5E15.5)
      IF(NPUNCH)3060,3030,3020
3020  WRITE(6,3025) (E(I),          DBIS(I),SIGT(I),I=NEDU,NEDL)
3025  FORMAT (1H$,1P3E12.5)
      GO TO 3030
 3060 CALL BCDUMP(E(NEDU),E(NEDL))
      CALL BCDUMP(DBIS(NEDU),DBIS(NEDL))
      CALL BCDUMP(SIGT(NEDU),SIGT(NEDL))
 3030 CONTINUE
      GO TO 1000
      END
$IBFTC EXPS1.  LIST
      FUNCTION EXPS1(XMIN,XMAX,FUNC1,KER)
      DIMENSION V(500),H(500),A(500),B(500),C(500),P(500),E(500),NE(500)
      EQUIVALENCE (E,NE),(TEST,NTEST)
      T=3.0E-5
      V(1)=XMIN
      H(1)=0.5*(XMAX-XMIN)
      C(1)=FUNC1(XMAX)
      B(1)=FUNC1(XMIN+H(1))
      A(1)=FUNC1(XMIN)
      P(1)=H(1)*(A(1)+4.0*B(1)+C(1))
      E(1)=P(1)
      ANS=P(1)
      N=1
      FRAC=2.0*T
    1 FRAC=0.5*FRAC
    2 TEST=ABS(FRAC*ANS)
      K=N
    3 DO 7 I=1,K
    4 IF(NTEST-IABS(NE(I)))5,5,7
    5 N=N+1
      V(N)=V(I)+H(I)
      H(N)=0.5*H(I)
      A(N)=B(I)
      B(N)=FUNC1(V(N)+H(N))
      C(N)=C(I)
      P(N)=H(N)*(A(N)+4.0*B(N)+C(N))
      Q=P(I)
      H(I)=H(N)
      B(I)=FUNC1(V(I)+H(I))
      C(I)=A(N)
      P(I)=H(I)*(A(I)+4.0*B(I)+C(I))
      Q=P(I)+P(N)-Q
      ANS=ANS+Q
      E(I)=Q
      E(N)=Q
    6 IF(N-500)7,13,13
    7 CONTINUE
    8 IF(N-K)9,9,2
    9 Q=0.0
   10 DO 11 I=1,N
   11 Q=Q+E(I)
   12 IF(ABS(Q)-T*ABS(ANS))14,14,1
   13 KER=KER+1
   14 ANS=0.0
   15 DO 16 I=1,N
   16 ANS=ANS+P(I)
      EXPS1=(ANS+Q/30.0)/3.0
```

```
   17 RETURN
      END
$IBFTC DBO.     LIST
      FUNCTION DBO(XX)
      COMMON NLEV,I,J,Z,CON,DBI,E,SIGC,SIGS,SIGF,ITYPES,NEDU,NEDL
      COMMON XMAX,KSAV
      DIMENSION E(2200),SIGC(2200),SIGS(2200),SIGF(2200)
      X=XX
      DO 2300 K=KSAV,NLEV
      IF(E(K)-X)2050,2300,2300
 2050 GO TO (2060,2070,2080),J
 2060 SIGM=SIGC(K)
      SIGN=SIGC(K-1)
      GO TO 2100
 2070 SIGM=SIGS(K)
      SIGN=SIGS(K-1)
      GO TO 2100
 2080 SIGM=SIGF(K)
      SIGN=SIGF(K-1)
 2100 CONTINUE
      EM=(SIGM-SIGN)/(E(K)-E(K-1))
      B=SIGM-EM*E(K)
      SIGX=EM*X+B
      ARG1=-Z*((SQRT (E(I))-SQRT (X))**2)
      ARG2=-Z*((SQRT (E(I))+SQRT (X))**2)
      P1 = EXP(ARG1)
      P2 = EXP(ARG2)
      DBO=((CON/E(I))*SQRT(X)*SIGX)*(EXP(ARG1)-EXP(ARG2))
      IF (X.EQ. XMAX) KSAV=K-1
      GO TO 2350
 2300 CONTINUE
 2350 CONTINUE
      RETURN
      END
$DATA
```

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TABLE I. - DOPPLER COEFFICIENTS FOR GOLD 197

Square root of surface to mass ratio, $\sqrt{S/M}$	Doppler coefficients, α				Effective resonance integral, I_{eff}
	Monte Carlo	Experimental	ZUT	TRIX	
1.30	[a] 4.06×10^{-5}	[b] 3.15×10^{-5}	4.31×10^{-5}	[b] 3.49×10^{-5}	130
	---	4.95	---	3.95	---
2.85	3.99×10^{-5}	[b] 3.21	3.69×10^{-5}	[b] 3.41	270
	---	3.45	---	2.90	---
6.02	6.34×10^{-5}	---	5.35×10^{-5}	5.00	550
6.99	6.93	---	6.08	5.35	610
9.89	7.06	---	6.71	5.60	800
11.4	6.93	[b] 4.62×10^{-5}	6.65	5.62	868
14.0	5.69	4.70	---	4.80	990
25.4	[c] 4.27	---	3.26×10^{-5}	2.75	1286
42.5	[c] 1.98	3.75×10^{-5}	1.61	1.30	1465

[a] This Monte Carlo value is corrected to allow for an upper cutoff of 500 eV (J) used. The value of ΔI_{eff} to this energy was 3.13, which represents only 77 percent of the total.

[b] These values are from ref. 11. All other experimental and TRIX values are from ref. 12.

[c] The effect of different cross-section sets was observed by rerunning each case with the ZUT agreement (see table II).

TABLE II. - MONTE CARLO AND ZUT RESULTS FOR IDENTICAL CROSS-SECTION SETS

Square root of surface to mass ratio, $\sqrt{S/M}$	Monte Carlo		ZUT		Difference, percent
	Change in effective resonance integral, ΔI_{eff}	Effective resonance integral, I_{eff}	Change in effective resonance integral, ΔI_{eff}	Effective resonance integral, I_{eff}	
25.4	10.05	-------	10.3	-------	2.4
	-----	1163.43	-----	1183.7	1.7
42.5	5.64	-------	5.72	-------	1.35
	-----	1321.72	-----	1331.67	.75

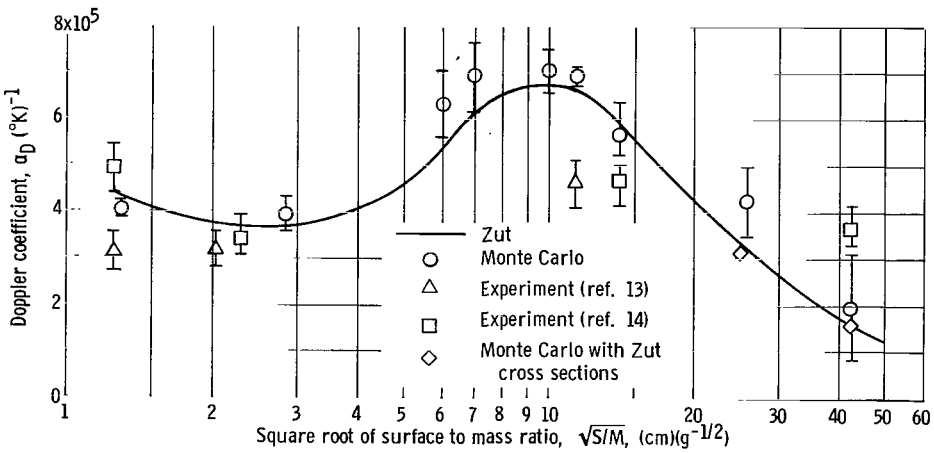

Figure 1. - Calculated and experimental values of Doppler coefficients as function of square root of surface to mass ratio.

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