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APPLICATIONS OF MONTE CARLO ANALYSIS TO TUNGSTEN RESONANCE ABSORPTION

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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ABSTRACT

Calculational procedures for Monte Carlo analyses and W resonance absorption are presented. The widely used flat spatial neutron source assumption is shown to overestimate the effective resonance integral of the large scattering resonance in W^{186} by 21 percent at a surface to mass ratio (S/M) of $0.5 \text{ cm}^2/\text{g}$. Resonance overlap in natural W decreases the effective resonance integral by 18 to 7 percent over a S/M range of 0.16 to $4.0 \text{ cm}^2/\text{g}$ relative to calculations which ignore resonance overlap. Spatial self-shielding in a complex geometric cell is evaluated through comparison of Monte Carlo calculations with exact geometric and homogenized absorber region representations. The code EPIGRAM, which selects energy points for resonance cross sections, is reported.

CONTENTS

	Page
SUMMARY	1
INTRODUCTION	2
TUNGSTEN CROSS SECTIONS	3
Resonance Parameters	3
Data Preparation	3
CALCULATIONAL PROCEDURE OF THE DRAMA PROGRAM	4
Calculational Geometry	5
Neutron Slowing Down Treatment	6
Statistical Accuracy	7
THE FLAT SPATIAL NEUTRON SOURCE APPROXIMATION	8
RESONANCE OVERLAP IN NATURAL TUNGSTEN	11
SPATIAL SELF-SHIELDING OF RESONANCE ABSORPTION IN A TUNGSTEN FUEL ELEMENT OF COMPLEX CYLINDRICAL GEOMETRY	12
CONCLUSIONS	15
APPENDIX - COMPUTER PROGRAM EPIGRAM	16
General Description	16
Input Instructions	20
FORTRAN Listing	22
REFERENCES	45

APPLICATIONS OF MONTE CARLO ANALYSIS TO TUNGSTEN

RESONANCE ABSORPTION

by Robert M. Westfall

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SUMMARY

Accurate calculation of capture rates in tungsten isotopes is required for reactors using tungsten as a structural or shielding material. Widely used analytical procedures employ approximations in calculating resonance escape probabilities for arbitrary geometric configurations or for calculating effective resonance integrals. The accuracy of these approximations is evaluated for three cases by the Monte Carlo method. The first case estimates the validity of the flat spatial neutron source assumption used in computing collision probabilities for absorbers as applied to the large 18.83-eV scattering resonance in tungsten 186. The use of the flat source approximation results in an overestimation of resonance absorption that varies widely with absorber lump size and with the magnitude of scattering and absorption resonance half widths.

The second case demonstrates the effect of ignoring resonance overlap among the isotopes of natural tungsten. Comparison of the calculated values with and without resonance overlap show that neglect of overlap for natural tungsten overestimates the effective resonance integral by 18 to 7 percent over a surface to mass ratio range of 0.16 to 4.0 square centimeters per gram.

The third application is a demonstration of how the detailed geometry treatment by the Monte Carlo method can significantly affect the resonance absorption in a complex cylindrical tungsten fuel element. Monte Carlo calculations of the resonance escape probability for such a fuel element show a significant difference in absorption probabilities between calculations which represent the absorber materials in discrete geometry or as a homogenized central smeared region.

As part of the procedures, presentation is made of the computer code EPIGRAM which provides zero temperature, Breit-Wigner, single level cross sections (the cross sections are Doppler broadened with another code) at those energy points from which the intermediate cross sections can be interpolated within prescribed absolute and percentage deviations. The resultant minimum number of cross sections at assured interpolational accuracies improve both the speed and the reliability of subsequent Monte Carlo calculations using the DRAMA code.

INTRODUCTION

The refractory properties of tungsten (W) make it a desirable material for use in high temperature reactors. However, the presence of large neutron absorbing resonances and their associated high thermal cross sections in the isotopes W^{182} , W^{183} , and W^{186} precludes the use of natural tungsten in thermal reactors for nuclear propulsion. It has been suggested (ref. 1) that tungsten enriched in the isotope W^{184} , which has a small resonance absorption integral and a low thermal absorption cross section, would be applicable. Since the cross sections of a mixture highly enriched in the W^{184} isotope would be dependent upon the residual absorbing isotopes, an accurate method for calculating resonance absorption in all isotopes is required.

Some widely used methods of treating resonance absorption (refs. 2 to 4) have been applied with accuracy to materials with widely spaced, predominantly absorbing resonances such as uranium 238. Under these conditions, the analytical treatment conveniently and validly assumes a flat spatial neutron source through the absorber region to compute collision probabilities and also complete energy flux recovery between adjacent resonances. These assumptions may not apply to tungsten because several of the tungsten resonances are closely spaced and have large resonance scattering widths. The Monte Carlo method can calculate resonance absorption without requiring these assumptions since this method has the advantage of following the slowing down of the neutrons as discrete particles.

The procedures described in this report have required the compilation of resonance parameters for the tungsten isotopes, the development of computer codes for the calculation of cross sections, and the calculation of effective resonance integrals and resonance escape probabilities with the Monte Carlo code, DRAMA (ref. 5).

Three cases of resonance absorption are studied with the Monte Carlo method. The first case is an evaluation of the error associated with the use of the flat spatial neutron source assumption in analyzing absorption by the large 18.83-eV scattering resonance of W^{186} . The second case is an evaluation of the effects of resonance overlap present in natural tungsten over a surface to mass ratio range of 0.16 to 4.0 square centimeters per gram. The third case studied is that of spatial self-shielding in a complex cylindrical tungsten fuel element. Detailed consideration of exact cell geometry relative to a homogenized absorber region representation results in a significantly lower value of the cell resonance absorption probability.

The appendix contains a description of EPIGRAM, a computer code developed to identify the energy points required to provide the minimum number of resonance cross sections at given interpolational accuracies. Additionally, the code provides the cross section arrays and the resonance absorption integral at infinite dilution. Operating instructions, a FORTRAN listing, and a sample problem are presented.

TUNGSTEN CROSS SECTIONS

Resonance Parameters

The accuracy of the Monte Carlo calculation is dependent upon the precision of the cross sections of the constituent materials and the completeness with which the cross sections are sampled over the energy spectrum. The resonance parameters for the tungsten isotopes have been remeasured in the last several years (refs. 6 to 10). Also, recent measurements on isotopically enriched tungsten samples have provided more accurate values of the isotopic-thermal absorption cross sections (ref. 11) and the infinitely dilute resonance integrals of W^{184} and W^{186} (ref. 12).

The compilation of tungsten resonance parameters (listed in the natural tungsten sample problem in the appendix) has been drawn primarily from the Oak Ridge National Laboratory - Rensselaer Polytechnic Institute measurements of the last few years. The main source is reference 6 from which parameters for all resonances above 87.4 eV are taken. Values for the low energy resonances were selected on the basis of consistency with reference 6. The sources of the low energy data are as follows. The first two resonances in W^{182} and the first resonance in W^{183} are from reference 7. For W^{183} , the second resonance is from reference 8, the third from reference 6, and the fourth, fifth, and sixth are from reference 9.

The bound level resonances in W^{182} and W^{184} have energies which were assigned to make up the differences between the measured thermal cross sections of reference 11 and the values calculated from the known parameters. The bound levels are based on the average neutron width and the assumed capture width of reference 6.

Parameters for the important first resonance in W^{186} are taken from reference 12 which compared absorption integrals calculated with various capture half widths with a precise measurement of the dilute resonance integral.

W^{180} has a very small natural abundance (0.0013); and it was not until an enriched sample (0.0693) became available that experimental measurements could be made. Thus the five resolved resonances of reference 10 constitute all the present information on this isotope.

Calculations of the thermal cross sections and dilute resonance integrals based on these parameters have been made for the tungsten isotopes. These are tabulated in the sample problem in the appendix and are compared with experimental values.

Data Preparation

In the Monte Carlo calculation, there is a choice of calculating Doppler broadened cross sections after each neutron collision or of energy interpolating the values from

tables of precalculated cross sections. Of the two methods, the interpolation technique is much faster. Since a typical calculation contains several hundred thousand neutron collisions, time becomes an important factor and the interpolation scheme is usually employed. The main area for concern with the interpolation scheme is that the tabulated energies must be chosen such that the cross sections can be interpolated between them with the desired degree of accuracy. For this purpose the computer code EPIGRAM was developed.

This code, which is discussed in detail in the appendix, provides zero temperature, Breit-Wigner, single level cross sections. The cross sections are Doppler broadened through the use of the DBCS code described in reference 13. Tables of cross sections for the separate nuclides, along with the corresponding energy tables, are entered into the DRAMA code for the Monte Carlo calculation. After each neutron collision, the DRAMA code ascertains the interacting nuclides, interpolates the cross sections semi-logarithmically in energy (see the appendix), and multiplies the cross sections by the proper number densities. Thus, the probabilities for the various events over the neutron energy spectrum are provided by a method which has sufficient speed, desirable flexibility, and assured accuracy.

CALCULATIONAL PROCEDURE OF THE DRAMA PROGRAM

The DRAMA program uses Doppler broadened cross sections to calculate the resonance escape probabilities of configurations of interest. Since it directly affects reactor criticality, the resonance escape probability p is an important parameter of the fuel cell configuration. The resonance escape probability is a function of the effective resonance integral. For a given material, the effective resonance integral I_{eff} is a measure of the integrated absorption probability over a specified energy range. Since the effective resonance integral varies primarily with the surface to mass ratio, it is an important parameter with which absorbing materials can be compared.

The procedure followed in this study has been to calculate the resonance escape probabilities of either complex fuel cell configurations or simple absorber geometries, obtaining the effective resonance integral through the following expression:

$$p = \exp\left(\frac{-N_A V_A I_{\text{eff}}}{V_M \overline{\xi \Sigma}_s}\right) \quad (1)$$

where N_A is the atom density of the absorber, $\overline{\xi \Sigma}_s$ is the average slowing down power

of the moderator, and V_A and V_M are the volumes of the absorber and moderator, respectively.

Calculational Geometry

The DRAMA program considers a geometry which is based upon an absorber-moderator cell. Upon intersecting the outer cell boundary, the neutrons' coordinates are adjusted so that they re-enter the cell in the same relative position that they would enter the adjacent cell of an infinite repetitive array. The outer cell boundaries may be cylindrical, rectangular, or hexagonal. The cells may be bounded by planes in the vertical direction. The internal cell boundaries, separating regions of constant material composition, can take any shape described by a first or second degree equation. The present version of the code can consider up to eight materials in any of the 30 internal regions. The program is limited to 15 materials overall, six of which can be resonance absorbers. A further limitation is the total of 50 internal and external boundaries used to describe the cell.

Resonance escape probabilities have been calculated for complex two-dimensional hexagonal cells containing concentric cylindrical regions, an example of which is shown

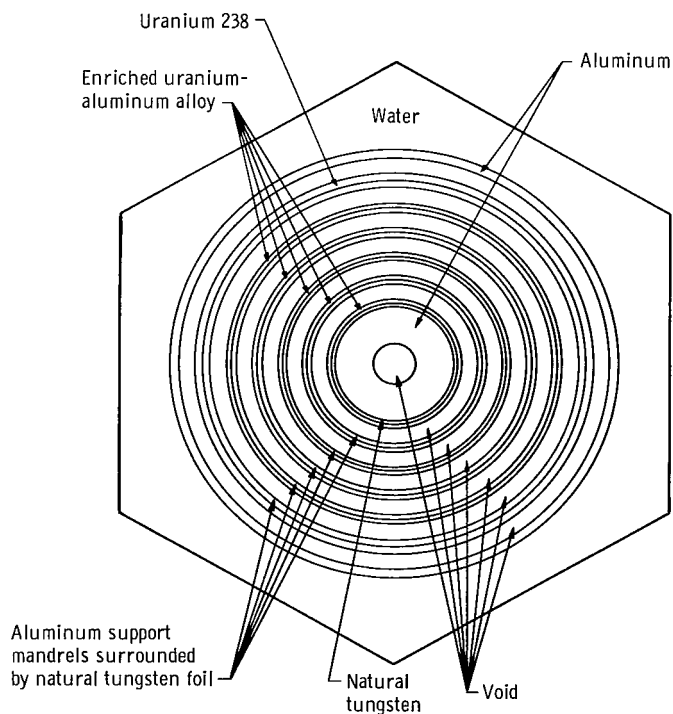


Figure 1. - Cross-sectional view of complex cylindrical tungsten fuel element.

in figure 1. Radial and axial leakage can be calculated by placing thick regions of "black" absorbing material adjacent to the outer cell boundaries.

When the calculational objective was obtaining effective resonance integrals, the slab lattice model shown in figure 2 was used. This simple model is easy to set up and

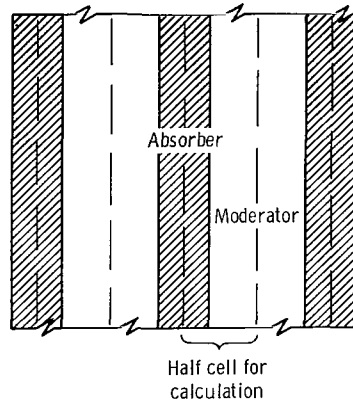


Figure 2. - Slab cell model in semiinfinite lattice.

does not require long running times for results of acceptable statistical quality. Symmetry conditions allow calculation of the half cell. Reflective cell boundary conditions restrict the surface of the absorber to a single plane. For a given absorber density ρ_A (g/cm^3), the absorber thickness τ (cm) is related to the desired surface to mass ratio S/M (cm^2/g) through the following expression:

$$\tau = \frac{2}{\rho_A(S/M)} \quad (2)$$

A procedure used to reduce running time was to minimize the moderator thickness. Minimum moderator thicknesses for maintaining an unperturbed neutron flux distribution, that is, a $1/E$ neutron flux, were established for several absorber material configurations.

Neutron Slowing Down Treatment

The DRAMA program employs a rejection technique to select the initial neutrons from an assumed $1/E$ neutron flux distribution over the energy interval between the maximum energy for the calculation and the minimum energy resulting from a single

elastic collision with the moderator atom.

Since inelastic scattering and p-wave and higher l -wave resonances are ignored in the calculation of the cross sections, the maximum energy should not exceed several thousand electron volts. An initial statistical weight of one is assigned to each neutron. This is reduced by the absorption probability over the neutron path length as it is scattered down in energy. The scattering is isotropic in the center of mass coordinate system. Each history is followed until its statistical weight falls below 0.00001 or the neutron's energy falls below the cutoff for the calculation. Since upscattering is ignored, the cutoff energy should be in excess of $5 kT$ where k is Boltzmann's constant and T is the temperature of the medium in $^{\circ}\text{K}$.

Statistical Accuracy

Calculation of the probable error has been used to determine the statistical accuracy as a function of the number of neutron histories. The resonance escape for the Monte Carlo calculation is defined as the sum of the terminal neutron weights ω_i divided by the number of neutron histories H . The variance of the resonance escape $V(p)$ is the second moment of p minus the square of the first moment; that is,

$$V(p) = \sum_i \frac{\omega_i^2}{H} - \frac{\left(\sum_i \omega_i\right)^2}{H^2} \quad (3)$$

The probable error $PE(p)$ is calculated as, in reference 14,

$$PE(p) = 0.6745 \sqrt{\frac{V(p)}{H - 1}} \quad (4)$$

There is a 50 percent expectation that the correct resonance escape value lies within $\pm PE(p)$. To increase the expectation, the appropriate coefficient taken from a table of the normal distribution function must be substituted. For ten thousand neutron histories, the probable errors of the resonance escape values run from 0.5 percent for high p values ($p > 0.95$) to 1 percent for low p values ($p < 0.85$). Since the effective resonance integral has a logarithmic dependence upon the resonance escape, the associated probable errors vary in the opposite direction. Typically, they vary from 2 percent for thin, moderately absorbing samples to 1 percent for thick, highly absorbing samples. It

should be noted that the thick samples have lower effective resonance integrals so that in absolute terms their associated probable errors are usually much less than those of thin samples. This indicates the increased difficulty of adequately sampling thin absorbers.

THE FLAT SPATIAL NEUTRON SOURCE APPROXIMATION

The flat spatial neutron source approximation, as applied in the Nordheim integral method of reference 2 to calculate collision probabilities, was early recognized to cause an overestimation of the resonance absorption for thick lumps of material with high ratios of resonance scattering to absorption (ref. 15). The validity of the flat source approximation for the large 18.83-eV scattering resonance in W^{186} has been studied by Cohen (ref. 16) using transport calculations.

The present Monte Carlo calculations were applied to the same problem to determine how the effective resonance integral varies with both absorber lump size and the ratio of scattering to absorption. The procedure involved a comparison of ZUT (ref. 4), which uses the flat source approximation, and DRAMA calculations of the effective resonance integral arising from the single 18.83 eV resonance. Consideration of the single resonance precludes the effect of resonance overlap as a complicating factor. A range

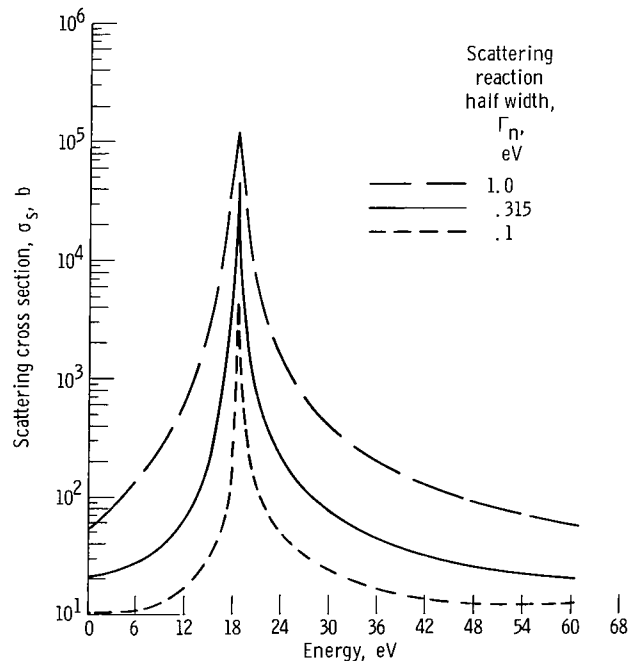


Figure 3. - Scattering cross section against energy for 18.83 eV resonance. Capture reaction half width $\Gamma_\gamma = 0.052$ eV; temperature $T = 300^\circ$ K.

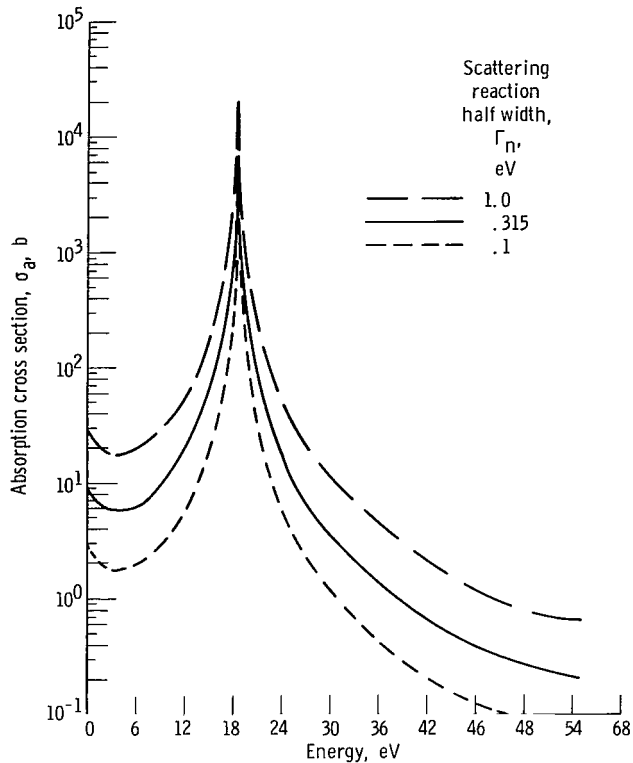


Figure 4. - Absorption cross section against energy for 18.83 eV resonance. Capture reaction half width $\Gamma_\gamma = 0.52$ eV; temperature $T = 300^\circ$ K.

of S/M values from 0.125 to 1.125 square centimeters per gram was considered. The ratio of scattering to absorption was varied by using scattering half widths of 1.0, 0.315, and 0.1 eV with a constant capture half width of 0.052 eV.

Both the Monte Carlo and ZUT calculations were based on the slab cell geometry. In the Monte Carlo calculation, 4 inches (10.16 cm) of water separating the absorber regions maintained a $1/E$ flux incident on the slabs. The atom density of W^{186} in the slabs was based upon a physical density of W^{186} of 19.3 grams per cubic centimeter. The energy range considered was between 100 and 8.07 eV (the $3/7 E_0$ cutoff of the ZUT calculation).

The 600 energy point, Breit-Wigner, single level cross sections of the Monte Carlo calculation were Doppler broadened to 300° K with the same shape functions used in the ZUT calculation. The scattering and capture cross sections for the actual and for extreme neutron widths are plotted in figures 3 and 4. It is seen that for the scattering cross section, both the peak value and the resonance width vary directly as the neutron width. Although the peak value of the capture cross section varies inversely as the neutron width, the integrated absorption probability over the resonance varies directly.

TABLE I. - COMPUTED RESONANCE INTEGRALS OF W^{186}
 BETWEEN 100 AND 8.07 eV

[Resonance energy $E_0 = 18.83$ eV; capture reaction half width
 $\Gamma_\gamma = 0.052$ eV; temperature $T = 300^0$ K; density
 $\rho = 19.3$ g/cm³.]

Scattering reaction half width, Γ_n , eV	Type of calculation	Surface to mass ratio, S/M, cm ² /g		
		0.125	0.5	1.125
0.1	I (ZUT) [†]	9.83	20.63	30.52
	I (Monte Carlo) [†]	9.05±0.35	19.68±0.98	30.02±1.8
	I_Z/I_{mc}^*	1.09	1.04	1.02
0.315	I (ZUT) [†]	15.58	33.96	51.08
	I (Monte Carlo) [†]	12.56±0.43	28.02±1.14	45.8±2.2
	I_Z/I_{mc}^*	1.24	1.21	1.11
1.0	I (ZUT) [†]	21.6	52.98	81.71
	I (Monte Carlo) [†]	12.97±0.45	42.45±1.55	64.34±3.1
	I_Z/I_{mc}^*	1.67	1.24	1.27

[†]Resonance integral in barns.

* $I_Z/I_{mc} = I (ZUT)/I (Monte Carlo)$.

The results of the study of the flat neutron source approximation are given in table I. Each of the Monte Carlo values represents 10 000 neutron histories, and the probable errors shown reflect their statistical accuracy. For a neutron width of 0.1 eV (on the same order as the capture width), the ZUT values do not seriously overestimate the effective resonance absorption integral. However, the dependence of the overestimation on absorber lump size is clearly seen. At the neutron width of 0.315 eV which corresponds to measured values of the actual resonance, the overestimation is seen to be in excess of 20 percent in the range of S/M values which are found in many reactor applications. The extreme case of the neutron width of 1.0 eV illustrates very large overestimations of I_{eff} by the ZUT calculation.

Cohen in reference 16 compared transport calculations employing a fine spatial mesh and 48 energy groups with calculations done with the ZUT code. Analysis was done on the effective resonance absorption integral of the same 18.83-eV level in W^{186} using a scattering half width of 0.317 eV and an energy range of 10.38 to 27.85 eV. An effective resonance absorption integral overestimation of 13 percent at S/M = 1.0 square centimeter per gram agrees closely with the 11 percent value at a S/M value

of 1.125 square centimeter per gram in table I. However, with the substitution of a hyperbolic cosine neutron distribution in the absorber region to compute the escape probability values as used by the ZUT code, Cohen has shown that the Nordheim integral method can be used to accurately calculate resonance absorption in thick slab geometries of highly scattering materials.

RESONANCE OVERLAP IN NATURAL TUNGSTEN

A commonly used assumption is that resonances are sufficiently spaced in energy to allow the complete recovery of the incident neutron flux to a $1/E$ distribution and thus do not interfere with each other. Natural tungsten has several closely spaced, large resonances in which overlap does occur. The present Monte Carlo calculations were made to determine the magnitude of the overlap effect in natural tungsten for a series of $\sqrt{S/M}$ values from 0.4 to 2 centimeters per gram^{1/2} (S/M varies from 0.16 to 4.0 cm²/g).

The effective resonance integrals were computed for samples of natural tungsten and for the four principal tungsten isotopes, W^{182} , W^{183} , W^{184} , and W^{186} at natural abundances. The overlap effect was estimated from the comparison of the value calculated for the natural tungsten with the sum of the values calculated for the constituent isotopes separately.

A repetitive slab lattice of alternate tungsten-water regions was used in the calculations. Two inches (5.08 cm) of water was sufficient to eliminate cell interaction effects. Six hundred energy point sets of Breit-Wigner, Doppler broadened (300° K) cross sections described each isotope. The energy range considered was from 2200 to 0.5 eV. The cross sections were calculated using resonance parameters available prior to the publication of reference 6; however, these are essentially the same as those found in the appendix. Atom densities for the isotopes were based on a tungsten density of 19.3 grams per cubic centimeter. Each calculation included 10 000 neutron histories except for the thin sample case, $\sqrt{S/M} = 2.0$ centimeters per gram^{1/2}, which required 20 000 histories for acceptable statistical accuracy. The probable errors of the Monte Carlo method vary from 1.3 percent for $\sqrt{S/M} = 0.4$ centimeter per gram^{1/2} to 2.5 percent for $\sqrt{S/M} = 2.0$ centimeters per gram^{1/2}.

Figure 5 shows the Monte Carlo effective resonance integrals for natural tungsten as calculated for the natural isotopic mixture and as the sum of contributions of separated, noninteracting isotopes. Also shown in figure 5 are experimental epicalcium effective resonance integrals (ref. 17). The Monte Carlo natural mixture results and the experimental results are seen to be in reasonable agreement. Inclusion of self-shielded unresolved resonance contributions of 0.5 to 1.5 barns as calculated by the TUZ code

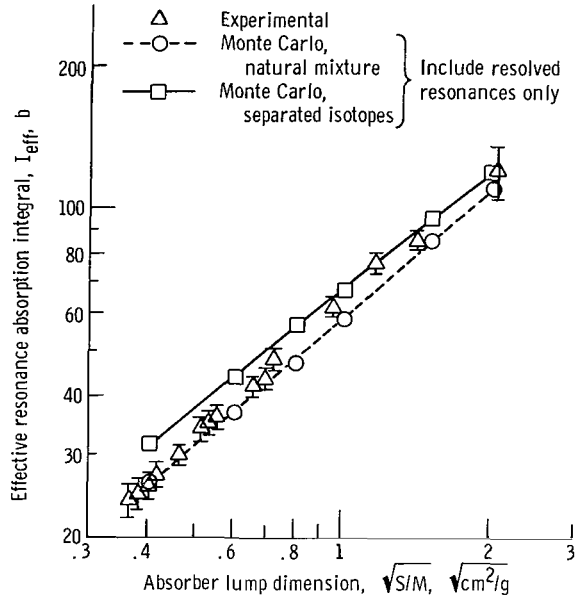


Figure 5. - Natural tungsten effective resonance integrals.

(ref. 4) in the Monte Carlo values for the range of $\sqrt{S/M}$ improves the agreement slightly.

Comparison of the Monte Carlo values in figure 5 shows the overlap effect to vary from 18 percent at $\sqrt{S/M} = 0.4$ centimeter per gram^{1/2} to 7 percent at $\sqrt{S/M} = 2.0$ centimeters per gram^{1/2}. By tabulating the absorptions between prescribed energy points in the Monte Carlo calculations it was possible to determine where the overlap occurs. For all values of $\sqrt{S/M}$, 80 percent or more of the overlap effect is attributable to the interaction of W^{186} and W^{182} which have large resonances at 18.83 and 21.09 eV, respectively. For the thicker samples, less than 10 percent of the overlap effect occurs in the $1/v$ region above 0.5 eV.

The Nordheim integral method has been extended in the GAROL code (ref. 18) to account for resonance overlap in calculating effective absorption cross sections. Calculations of W^{182} , W^{183} , and W^{186} between 2.38 and 61.4 eV show overlap effects of 6.5, 1.2, and 9.3 percent, respectively (ref. 19).

SPATIAL SELF-SHIELDING OF RESONANCE ABSORPTION IN A TUNGSTEN FUEL ELEMENT OF COMPLEX CYLINDRICAL GEOMETRY

This section illustrates the calculation of the resonance escape probability for a complex cylindrical fuel element and demonstrates that the spatial self-shielding can be

precisely accounted for by the Monte Carlo method. The capability of the DRAMA code to represent the internal and external boundaries of the lattice cell has already been discussed. This capability, coupled with the Monte Carlo method's continuous treatment of the phase space, permits an exact geometrical representation in the neutron slowing down calculation. Thus the Monte Carlo method has an inherent advantage over more approximate methods in calculating the spatial self-shielding of resonance absorption in a multiple region cell. The present study is of an experimental fuel element (ref. 19). The effects of the spatial self-shielding is shown through comparison of Monte Carlo calculations containing discrete and smeared representations of the annular absorber regions. The resonance escape value derived from a multigroup neutron transport calculation of the same fuel element is discussed qualitatively in the light of the Monte Carlo findings.

The fuel element geometry is shown in figure 1. Detailed compositions and dimensions of the material regions can be found in reference 19. Briefly, the overall pitch of the lattice cell is 7.62 centimeters. The 0.165-centimeter outer aluminum pressure tube has an outer diameter of 6.5 centimeters. Resting on five aluminum support mandrels and an inner support tube are six subassemblies. The inner five subassemblies have 0.0127 centimeter of natural tungsten surrounded by 0.1067 centimeter of 35 weight percent uranium (93.5 percent U^{235}) - aluminum alloy. The outermost subassembly has 0.762 centimeter of natural tungsten surrounded by 0.1016 centimeter of depleted uranium (0.22 percent U^{235}).

The geometrical model used in the Monte Carlo calculations was the same as that shown in figure 1 with the exception that the inner void was smeared into the thick aluminum support tube. This results in a 30 region geometry, the present capacity of DRAMA. Calculations were of the quarter cell in the x-y plane. Each of the six resonance absorbers (four isotopes of tungsten, two of uranium) were entered discretely. They were represented by 600 energy point tables of Breit-Wigner, single level cross sections Doppler broadened to 300° K. The calculations included a slowing-down energy range from 2034.68 to 0.532 eV.

The resonance escape probability for the discrete geometry model was calculated to be 0.708. This value represents 6000 neutron histories and it has an associated probable error of 0.003. The smeared geometry contained two regions, the water moderator and the remainder of the cell. The resonance escape probability after 6000 histories was 0.691 with a probable error of 0.002. The absorption in the cell during slowing down is therefore 5.5 percent greater for the smeared case than for the case with the discretely represented geometry.

Current methods of reactor analysis involve the use of the multigroup S_n transport calculation to determine the reactor multiplication factor. The general procedure is to consider the fuel element and its surrounding moderator as a cell in an infinite lattice.

Material cross sections are prepared with cross section averaging programs such as GAM II (ref. 20). Using an S_n transport program such as TDSN (ref. 21) and the material cross sections, a cell calculation is performed to obtain flux weighted cell cross sections. The flux weighted cell cross sections are then used in a transport calculation of the full reactor core to determine the multiplication factor.

The cell transport calculation corresponds to the Monte Carlo calculation described previously. It is of interest to derive the resonance escape probability from the cell calculation and compare it to the Monte Carlo value. However, only a qualitative comparison can be made because of several approximations inherent in both the cross section averaging and the cell calculation.

A 16 energy group S_4 , P_1 , one-dimensional transport calculation was done for the same cell geometry as that used in the discrete region Monte Carlo calculation. Ninety-nine mesh points were distributed over the 30 discrete material regions. The hexagonal outer cell boundary was approximated by the circle which conserves the area of the moderator.

The 16 energy groups of the material cross sections included four groups in the resonance energy region of the Monte Carlo calculations. The GAM II program was used to calculate 34 fine group resonance cross sections and flux weight them into the four broad groups. The calculation of the fine group cross sections is done with the ZUT-TUZ procedure. Three approximations are involved in this initial stage of the cross section preparation. The absorber materials are treated as a lumped region and thus spatial self-shielding is ignored. The escape probability table for the lumped absorber is based on the flat spatial neutron distribution approximation for a solid cylindrical rod. And each resonance nuclide is treated separately with resonance overlap not taken into account. The 34 fine group cross sections were flux weighted over a spectrum resulting from the interaction of fission spectrum neutrons with the cell materials to obtain the four broad group cross sections. Spatial self-shielding remains to be treated in the cell calculation.

The S_n cell calculation, in principle, could exactly account for spatial self-shielding if it contained an adequate number of mesh points. How well the 99 mesh points account for the spatial self-shielding cannot be determined quantitatively because of the approximations in the cross section preparation discussed previously and also because of several differences between the transport and Monte Carlo calculations.

The significance of the resonance overlap effect was shown by making Monte Carlo calculations of each resonance nuclide separately in the discrete region geometry. The resulting value of the resonance escape probability 0.608, reflects an absorption probability which is 39.2 percent greater than the value with resonance overlap taken into account.

The value of the resonance escape probability derived from the transport calculation

is 0.669. The difference between this value and the discrete region Monte Carlo value of 0.708 cannot be attributed entirely to resonance overlap and spatial self-shielding. In addition to the several effects discussed previously, minor effects could arise from the circular outer cell boundary approximation or the difference in the source neutron flux slowing down into the resonance region.

The Monte Carlo calculations have shown that the detailed representation of geometry results in an absorption probability which is 5.5 percent less than that of the smeared cell. It is probable that the transport cell calculation does not account for all of this effect. Significant differences have been shown between the S_n and Monte Carlo resonance absorption probabilities. The number of approximations in the S_n transport calculation demonstrates the desirability of the exact Monte Carlo method for cells of complex geometry.

CONCLUSIONS

The Monte Carlo method as applied to resonance analysis can account directly for effects which other methods treat approximately. The results of the Monte Carlo studies of three of these effects upon tungsten resonance absorption are summarized here.

The analytic approximation based on the assumption of a flat spatial neutron source distribution through the absorber leads to overestimations of resonance absorption in thick lumps of high resonance scattering material. The effective resonance absorption integral contribution of the large scattering resonance at 18.83 eV in W^{186} is overestimated by 21 percent at a surface to mass ratio of 0.5 square centimeter per gram when the flat spatial neutron distribution is employed.

Resonance overlap in natural tungsten reduces the effective resonance integral at low surface to mass ratios relative to calculations which superpose the isotopic capture rates. The overlap effect varies from 18 to 7 percent over a surface to mass ratio range of 0.16 to 4.0 square centimeters per gram.

Spatial self-shielding decreases the resonance absorption probability of a complex cylindrical tungsten fuel element by 5.5 percent. The resonance escape probability derived from a neutron transport calculation of the same fuel element is significantly less than the Monte Carlo value. The difference is attributed to a number of effects of which resonance overlap and spatial self-shielding are probably the most important, but the effects cannot be separated in the transport calculation.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, February 1, 1968,
129-02-04-03-22.

APPENDIX - COMPUTER CODE EPIGRAM

General Description

The purpose of the code is to generate zero temperature, Breit-Wigner, single level cross sections at those energy points which allow interpolation of intermediate cross sections at a desired degree of accuracy. The minimum number of energy points thus produced reduces computation time.

The procedure followed by the code is to cover the resonances with a large number of closely spaced energies. The corresponding cross sections are calculated. Then, by using the same interpolation technique applied in the Monte Carlo calculation, those energies at which the cross sections can be interpolated within the desired margins of absolute and percentage accuracies are eliminated.

The initial energy grid is generated upon the resonance base energies, the energies at one-half and two total widths off the base, and the wing points at which the total cross section is less than 0.0005 of the maximum. If the wing points of adjacent resonances overlap, they are reset at equal intervals between the corresponding points at two total widths off the base energies. The initial grid is expanded by equally spacing 19 additional points between each of the original points. The process results in a grid of $140N + 21$ energy points where N is the number of resonances.

Through iterative procedures, the code can consider a material containing as many as 1200 resonances. Ten is the maximum number of isotopes. Each of the two statistical weight factors g associated with each isotope can have as many as 60 resonances. If it is desired to have more than 60 resonances associated with one g factor, the isotope can be entered twice with the second entry containing the additional resonances in one or both of its g factors. In this instance, care must be taken to ensure the correct potential scattering contribution for the isotope by using a zero value for the potential scattering multiplying term PSTM of the second entry.

The code executes the interpolation and elimination-through-comparison scheme on the table of total cross sections. The zero temperature, Breit-Wigner, single level cross sections with interference between resonance and potential scattering taken into account are calculated according to the following formulas:

$$\sigma_S(E) = \sum_{in=1}^{NI} 4\pi B_{in} \left(\frac{A_{in} + 1.008986}{A_{in}} \right)^2 \left\{ \sum_{k=1}^2 g_k \left| \sum_{j=1}^{NR_k} \left[\frac{(\Gamma_{n,j}/2)\lambda_{r,j}}{(E - E_{O,j} + i\Gamma_j/2)} \right] - \lambda_E e^{-i\delta} \sin \delta \right|^2 \right\} \quad (A1)$$

$$\sigma_C(E) = \sum_{in=1}^{NI} \pi B_{in} \left(\frac{A_{in} + 1.008986}{A_{in}} \right)^2 \sum_{k=1}^2 g_k \lambda_E \sum_{j=1}^{NR_k} \frac{\Gamma_{n,j} \Gamma_{\gamma,j} \lambda_{r,j}}{(E - E_{O,j})^2 + (\Gamma_j/2)^2} \quad (A2)$$

$$\sigma_f(E) = \sum_{in=1}^{NI} \pi B_{in} \left(\frac{A_{in} + 1.008986}{A_{in}} \right)^2 \sum_{k=1}^2 g_k \lambda_E \sum_{j=1}^{NR_k} \frac{\Gamma_{n,j} \Gamma_{f,j} \lambda_{r,j}}{(E - E_{O,j})^2 + (\Gamma_j/2)^2} \quad (A3)$$

where

- A atomic mass
- B fractional atomic abundance
- E neutron energy, eV
- E_O resonance energy, eV
- g statistical weight factor
- i $\sqrt{-1}$
- NI number of isotopes
- NR number of resonances

R nuclear radius, $1.5 \times 10^{-13} A^{1/3}$, cm

Γ reaction half width, eV

δ $-2.196979 \times 10^9 R \sqrt{E}$

λ $\frac{2.86 \times 10^{-9}}{2\pi \sqrt{E}}$, cm

σ cross section, b

and the subscripts are

c, γ capture

E neutron energy applies

f fission

in isotope number

j resonance number

k g factor number

n, s scattering

r resonance energy applies

The interpolation may be done either semilogarithmically or linearly in energy. The semilogarithmic scheme requires more time but results in about 25 percent fewer points for the same degree of accuracy. The shorter table lookup time in the Monte Carlo calculation more than makes up for the longer interpolation time. Whichever scheme is selected, assured accuracy of the cross sections depends upon the consistency of their generation and application.

For energy points i, j, and k, the cross section at point j is interpolated as follows:

Semilogarithmic:

$$\sigma_j = \sigma_k \left(\frac{\sigma_i}{\sigma_k} \right)^{(E_k - E_j)/(E_k - E_i)} \quad (\text{A4})$$

Linear:

$$\sigma_j = \left(\frac{\sigma_k - \sigma_i}{E_k - E_i} \right) (E_j - E_i) + \sigma_i \quad (\text{A5})$$

Provision is made to eliminate progressive series of points j by advancing the index k and reinterpolating and comparing all points j . When a point j fails the tests, the k point corresponding to the preceding successful series of interpolations is retained to be printed out in the final array. Then the i index is advanced to this k value and the process continues.

When a point fails on its initial interpolation, that is, it must be retained, additional tests are made on the percent deviation to determine if the initial grid is too coarse between points i and k . The upper limit on the percent deviation is set at 10 percent except at those points where $\sigma_i + \sigma_j + \sigma_k < 2$ barns. At these points deviations up to 20 percent are allowed. If these upper limits are exceeded, intermediate points at successively finer intervals are inserted between points i and k . Cross sections are calculated and the interpolation tests are run until all of the intermediate points fall within the upper limit criteria. These points are retained, the i index is advanced to k , and the elimination of points from the original lattice is resumed.

Additionally, certain points of particular interest are retained. These are the maximum, minimum, and inflection points associated with the resonances. Inflection points are detected by monitoring the sign of the interpolated deviation. Maxima and minima are detected by comparing successive cross section values. Neither criteria is applied if a point is retained for exceeding the interpolated deviation.

Flexibility has been provided in the code to permit three irregular situations. The first is the inclusion of the contributions from bound level resonances at negative resonance energies. These are included in the input in the normal manner with the number of negative resonances NNR specified on the first control card. This results in their exclusion from the initial energy lattice, however, the subsequent cross section calculations do account for their contributions (by taking the absolute values of the resonance energies).

The second situation is one in which resonances of interest lie above or below the energy range of the problem. Resonances below the low energy cutoff EMN can be accounted for by using the NNR variable in the same manner described previously. Resonances above the high energy cutoff can be treated in the same way by specifying their total number NRSAEX on the first control card.

The third situation arises from resonances for which the spin state has not been determined. An average g factor value of one-half is used in resolving their parameters. This procedure has led to three effective g factors for these isotopes. Using the same technique as that employed in including more than 60 resonances for a single g factor value will allow the inclusion of these resonances; that is, by entering the isotope twice, using the $g = 1/2$ resonances in the second entry, and setting its potential scattering multiplying term equal to zero. An application of this procedure appears in the sample case. Use of the $g = 1/2$ resonances represents an approximation, and it can result in

excessive interference and small negative scattering cross sections in the s-wave dip of small resonances. Provision has been made to set these cross sections equal to 0.01 barn. The procedure is more accurate than ignoring the resonances or arbitrarily assigning spin states.

Finally, the code calculates the incremental contribution to the resonance absorption integral at infinite dilution. The contribution between energies E_1 and E_2 is calculated by applying the linear interpolation expression for the absorption cross section to the following formula:

$$\begin{aligned}
 \Delta I_{\infty}(E_1 \rightarrow E_2) &= \int_{E_1}^{E_2} \sigma_a(E) \frac{dE}{E} \\
 &= \int_{E_1}^{E_2} \left[\left(\frac{\sigma_2 - \sigma_1}{E_2 - E_1} \right) (E - E_1) + \sigma_1 \right] \frac{dE}{E} \\
 &= \left(\frac{\sigma_2 - \sigma_1}{E_2 - E_1} \right) \left[E_2 - E_1 \left(1 + \ln \frac{E_2}{E_1} \right) \right] + \sigma_1 \ln \frac{E_2}{E_1} \quad (A6)
 \end{aligned}$$

The printed output includes the retained energies with their cross sections and the corresponding dilute resonance integral. These are followed by an edit which contains information on how many of the points are retained under the various criteria and the average percent deviation of the discarded points. The energies and their cross sections are punched out on cards.

The program is written in the FORTRAN IV language. Running times on an IBM 7094 II vary from 0.1 minute for a five resonance problem to 15 minutes for a full energy grid containing 115 resonances. If a number of the resonances are above or below the energy grid, such as in the sample case, the running time is considerably reduced. A 27 resonance problem takes less than 2 minutes.

Input Instructions

I Problem Identification Cards

Alphanumeric information in card columns 3 to 72 will be printed previous to problem output. The last card must have a number in card column 1.

II Control Card

Quantity	Format	Card columns	Remarks
N	I10	1-10	Total number of resonances
NI	I10	11-20	Number of nuclides
FD	F10.5	21-30	Fixed difference between calculated and interpolated values allowed
PD	F10.5	31-40	Percentage difference between calculated and interpolated values allowed
EMN	F10.5	41-50	Minimum energy for output grid
EMX	F10.5	51-60	Maximum energy for output grid
INTYP	I5	61-65	= 0 Semilogarithmic interpolation will be used = 1 Linear interpolation will be used
NNR	I5	66-70	Number of resonances below EMN
NRSAEX	I5	71-75	Number of resonances above EMX
PCH	F5.0	76-80	= 0.0 No punched cards = 1.0 One set per card of energy, total, scattering, capture, and fission cross sections in Format 1P5E 12.5

III Data Card For Each Isotope (NI cards)

Quantity	Format	Card columns	Remarks
A	F10.5	1-10	Atomic mass number
AB	F10.5	11-20	Fractional abundance
R	E11.5	21-31	Nuclear radius (cm)
NGI	I9	32-40	Number of g factors associated with isotope (1 or 2)
PSTM	F10.5	41-50	Potential scattering term multiplier (1.0 unless isotope appears more than once, 0.0 for second entry)

IV Data Card For Each g Factor (two NI cards)

An extra blank card must be inserted for each isotope having only one g factor (see sample problem).

Quantity	Format	Card columns	Remarks
GL	F10.5	1-10	Value of g factor
NR	I10	11-20	Number of resonances associated with each g factor

V Data Card For Each Resonance (N cards)

Quantity	Format	Card columns	Remarks
EB	F10.5	1-10	Energy of resonance (eV)
NGTG	I10	11-20	Identification of g factor of resonance, g factors numbered in order of entry
GMNP	F10.5	21-30	Neutron scattering half width (eV)
GMGP	F10.5	31-40	Radiative capture half width (eV)
GMFP	F10.5	41-50	Fission half width (eV)

FORTRAN Listing

```

C
C      **** EPIGRAM ****
C
C      ENERGY POINT IDENTIFICATION AND CROSS SECTION GENERATION FOR
C      RESONANCE ABSORBING MATERIALS
C
C      COMPLEX ALGEBRA PROGRAMED BY MARY ANN ARNOLD, LEWIS RESEARCH CENTER
C
C      DIMENSION ER(505), SGSR(505), SGAR(505), SGFR(505), SGTR(505),
C      1ES(2750), SGS(2750), SGAS(2750), SGFS(2750), A(10), AB(10), R(10),
C      2G(10,2), EG(20,60), GMN(20,60), GMG(20,60), GMF(20,60), AR(20),
C      3GL(20), NRG(20), GI(10), COEF(10), P(501), ET(260), ST(260),
C      4SAT(260), SF1(260), EB(1200), GMNP(1200), GMGP(1200), GMFP(1200),
C      5NGTG(1200), NGI(10), ADRAI(505), PSTM(10), TITLE(14)
C      EQUIVALENCE (SGAS(1),NGTG(1)), (SGAS(1201), GMFP(1)), (SGAS(2401),
C      1GMGP(1)), (SAT(1), GMGP(351)), (SFT(1), GMGP(611))
C      COMPLEX DEN, EX1, T1, T2, CEX1, VAL3
C      WRITE(6,100)
C
C      READ AND WRITE TITLE CARDS
C
C      74 READ(5,113) NTITLE, (TITLE(I),I=1,14)
C      WRITE(6,114) (TITLE(I),I=1,14)
C      IF(NTITLE) 74,74,75
C
C      READ GENERAL INPUT

```

```

C
75 READ (5,1C1) N,NI,FD,PD,EMN,EMX,INTYP,NNR,NRSAEX,PCH 1E
   IF (INTYP)78,79,78
78 WRITE(6,115) 25
   GO TO EC
75 WRITE(6,116)

C
C   READ NUCLIDE DATA
C
8C READ (5,1C2) (A(I), AB(I), R(I), NGI(I), PSTM(I), I=1,NI) 27
   IGN= NI*2 2E

C
C   READ G FACTOR DATA
C
   READ (5,1C3) (GL(I),NR(I),I=1,IGN)

C
C   INITIALIZE PARAMETERS
C
C 35
   KO1 = C
   CKO2 = C.C
   NKST = C
   KC = C
   NK = 1
   KZ = C
   ICU = C
   NJ = C

C
C
C   ASSOCIATE G FACTORS WITH NUCLIDES
C
C
   DO 1 I=1,NI
   M=2*I
   MM=M-1
   G(I,1)= GL(MM)
1 G(I,2)= GL(M)

C
C   READ RESONANCE DATA
C
   READ (5,1C4) (EB(I),NGTG(I), GMNP(I), GMGP(I), GMFP(I), I=1,N)

C
C   ZERO COUNTER FIELD
C
C 65
   DO 2 I=1,IGN
2 NRG(I) = C

C
C   MATCH RESONANCE DATA WITH G FACTORS
C
C
   DO 3 I=1,N
   NT1= NGTG(I)
   NRG(NT1) =NRG(NT1)+1
   NT2= NRG(NT1)
   EO(NT1,NT2) = EB(I)
   GMN(NT1,NT2) = GMNP(I)
   GMG(NT1,NT2) = GMGP(I)
   GMF(NT1,NT2) = GMFP(I)
3 GMNP(I)= GMNP(I) + GMGP(I) + GMFP(I)

C
C   ZERO INITIAL TOTAL CROSS SECTION FIELD
C
   DO 21 I=1,2750
21 SGAS(I)=0.C

C
C   CALCULATE NUCLIDE CROSS SECTION COEFFICIENTS
C
C
   DO 4 J=1,NI
   AF = ((A(J) + 1.C08586)/A(J))**2
4 COEF(J) = AB(J)* AF*1.25663704E25

```

```

C
C      WRITE INPUT DATA BY NUCLIDE,G FACTOR,RESCNANCE
C
      DO 55 I=1,NI
      WRITE(6,110)
      AP=A(I)
      ABP=AB(I)
      RP=R(I)
      INC=NG1(I)
      DO 55 IG= 1,ING
      GP=G(I,IG)
      NF = I*2-2+IG
      NGR = NR(NF)
      DO 55 IN=1,NGR
      EP=EO(NF,IN)
      GMNW=GMN(NF,IN)
      GMGW=GMG(NF,IN)
      GMFW = GMF(NF,IN)
55 WRITE(6,111) AP, ABP, RP, GP, EP, GMNW, GMGW, GMFW
C
C      ZERC INTERMEDIATE CAPTURE AND FISSION FIELDS
C
      DO 25 I=1,260
      SAT(I)=C.C
25 SFT(I)=C.C
C
C
C      *** THROUGH 5, SET LP P ARRAY ON EO,1/2+2 GAMMA TCTAL OFF EO,
C      AND WING POINTS ***
C
C
      P(1)=EMN
      ND = 1+NNR
      IC=1
      J=1
C
C
C      LOOP THROUGH STATEMENTS 14,18 ON 83 RESCANCES AT A PASS
C
      NDES = N - NRSAEX
      IF(NDES.LT.83) GO TO 15
      MD = 83
      GO TO 16
15 MD = NDES
16 IC = IC + 1
      IF(ND.EQ.1+NNR) GO TO 17
      P(1) = P(J+1)
      J = 1
      NSK = C
17 DO 5 I=ND,MD
      IF(NSK.EQ.1) GO TO E2
      IF(EB(I).NE.EB(I+1)) GO TO E1
      IF(GMNP(I)-GMNP(I+1)) 82,83,83
82 NSK = C
      J = J-1
      GO TO 5
83 NSK = J
81 CT= GMNP(I)
      GT2= CT*GT
      GM=5.5
      WS=GM*CT
      EW= EB(I)-WS
      IF(EW-EMN) 57,57,566
57 P(J+1) = EMN + C.C5
      GO TO 5E
566 CR = (SQRT(EB(I)) * GT2)/(SQRT(EW) * (4.0*WS**2 + GT2))
      IF(CR.LT.0.0005) GO TO 7
      GM=GM+5.0
      GO TO 6

```

126

144

202 203

```

7 P(J+1) = EB(I) - WS
58 P(J+2) = EB(I) - 2.C*GT
P(J+3) = EB(I) - C.5*GT
P(J+4) = EB(I)
P(J+5) = EB(I) + C.5*GT
P(J+6) = EB(I) + 2.C*GT
P(J+7) = EB(I) + WS
5 J = J + 7
J = J - 1
IF(MD.NE.NDES) GO TO 8
IF(P(J+1).LE.EMX) GO TO 73
P(J+1) = EMX - 1.C
73 P(J+2) = EMX
J = J + 1

```

C
C
C
C
C

CHECK AND RESET IF WING POINTS OVERLAP

```

8 DO 9 IL = 2, J
L = IL - 1
IF(P(IL).GT.P(L)) GO TO 9
K = IL - 2
KI = IL + 1
DELP = (P(KI) - P(K))/3.C
P(L) = P(K) + DELP
P(IL) = P(L) + DELP
9 CONTINUE

```

C
C
C
C
C
C
C

*** THROUGH 12, EXPAND P ARRAY BY FACTOR OF 20 TO FORM INITIAL ENERGY ARRAY ***

```

LMN = J+1
D = 20.C
KIM = 20
KS = 1
KIC = 1

```

C
C
C
C
C

LOOP THROUGH STATEMENTS 26,13 ON 125 P POINTS AT A PASS

```

IF(J.LT.125) GO TO 10
KI = 125
GO TO 11
10 KI = J
11 J1 = C
KIC = KIC + 1
DO 12 I1 = KS, KI
DL = (P(I1+1) - P(I1))/D
DO 20 KIL = 1, KIM
X = FLGAT(KIL)
X1 = X - 1.C
MN = J1 + KIL
20 ES(MN) = P(I1) + X1*DL
12 J1 = J1 + KIM

```

C
C
C
C
C
C
C

*** THROUGH 22, CALCULATE INITIAL TOTAL CROSS SECTION ARRAY

```

NJ = MN + NJ
MN = MN + 1
ES(MN) = P(I1+1)

```

C
C

```

C      ENERGY LOOP
C
C
DO 22 I2 = 1,MN
SGS(I2) = 0.C
SGAS(I2) = 0.0
SGFS(I2) = 0.0
INCJ = 1
SREI= SQRT(ES(I2))

C
C
C      NUCLIDE LOOP
C
C
DO 22 IN = 1,NI
JIG = C
SGSP = C.C
SGAP = C.C
SGFP= C.C
DEL = -2.1566175E9 * R(IN) * SREI
WL = 4.551821E-10 / SREI
VAL2 = SIN(DEL)
EX1 = CMPLX(C.,-DEL)
CEXP1 = CEXP(EX1)
T2 = CEXP1 * VAL2 * WL
ABT2 = CABS(T2)
SGRI = 0.C
JI = INCJ+ NGI(IN) -1

C
C
C      G FACTOR LOOP
C
C
DO 23 IJ = INCJ, JI
SGAPR = 0.C
SGFPR = C.C
JIG = JIG + 1
NRES = NR(IJ)
T1 = C.C

C
C
C      RESONANCE LOOP
C
C
DO 24 N2 = 1,NRES
P1 = ES(I2) - EO(IJ,N2)
P2 = (GMN(IJ,N2) + GMG(IJ,N2) + GMF(IJ,N2))/2.
DEN = CMPLX(P1,P2)
DENSP = P1**2 + P2**2
BLAMR = WL * SREI/SQRT(ABS(EO(IJ,N2)))
SPCF = WL*BLAMR*GMN(IJ,N2)/DENSP
SGAPR = GMG(IJ,N2) * SPCF + SGAPR
SGFPR = GMF(IJ,N2) * SPCF + SGFPR
24 T1 = (GMN(IJ,N2) /2./ DEN)*BLAMR+T1
VAL3 = T1-T2
VAL1 = CABS(VAL3)
SGAP = SGAP + SGAPR * G(IN,JIG)
SGFP = SGFP + SGFPR * G(IN,JIG)
SGSP = SGAP + SGFP
22 SGRI = G(IN,JIG) * (VAL1**2 - ABT2**2) + SGRI
INCJ = INCJ + 2
SGS(I2) = COEF(IN)*(SGRI+PSTM(IN)*ABT2**2+SGSP/4.0) + SGS(I2)
SGAS(I2) = COEF(IN)/4.C * SGAP + SGAS(I2)
22 SGFS(I2) = COEF(IN)/4.C * SGFP + SGFS(I2)
IF(ES(1).NE.EMN) GO TO 56

C
C
C      FIRST OUTPUT POINT
C
C
NK = 1 + NK
ER(NK) = ES(1)
SGTR(NK) = SGS(1)
SGAR(NK) = SGAS(1)
SGFR(NK) = SGFS(1)
SGSR(NK) = SGS(1) - SGAS(1) - SGFS(1)

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299

305

306

307

323

330


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C
  CI = XC/ABS(XC)
  CIM = CI*CIL
  CIL = CI
  IF (CIM - 0.5) 32,33,33
C
C
C   CHECK FOR MAXIMUM,MINIMUM POINTS
C
C
32 IF(SGS(K) - SGS(I)) 34,34,35
34 IF(SGS(K) - SGS(L)) 32,30,30
35 IF(SGS(K) - SGS(L)) 30,30,32
30 CONTINUE
  KM = KM + 1
  CX = XC
  L = L + 1
  IF (L.GT.LEP) GO TO 31
C
C
C   RETURN FOR SUCCESSIVE ELIMINATION
C
C
GO TO 29
C
C   COUNTER ON MAX,MIN,INFLECTION
C
32 ICU = ICU + 1
31 IF (KM) 36,27,36
C
C
C   CHECK MAGNITUDE OF SIGMAS TO DETERMINE IMPORTANCE OF
C   PERCENTAGE DIFFERENCE AND SET UPPER LEVEL
C
C
37 IF(SGS(I) + SGS(K)+SGS(L)-2.C) 38,38,39
38 CP = 20.0
  GO TO 40
39 CP = 10.0
40 IF(PC.GT.DP) GO TO 41
C
C
C   RETAIN POINT, GO TO STORAGE
C
C
M = K
GO TO 42
C
C
C
41----50, CALCULATE INTERMEDIATE POINTS UNTIL UPPER LIMIT
CRITERIA IS MET THROUGHOUT. ENERGY INTERVAL IS DIVIDED BY
SUCCESSIVE POWERS OF 2 UNTIL STOPPED AT 256.
CROSS SECTION CALCULATION,INTERPOLATION AND COMPARISON
SEQUENCING ARE THE SAME AS ABOVE.
C
C
41 KJ = 2*KJ
  IF(KJ.LT.256) GO TO 43
  WRITE(6,107) ES(I),ES(L)
  GO TO 44
42 ET(1) = ES(I)
  ST(1) = SGS(I)
  SAT(1) = SGAS(I)
  SFT(1) = SGFS(I)
  ET(KJ+1) = ES(L)
  ST(KJ+1) = SGS(L)
  SAT(KJ+1) = SGAS(L)
  SFT(KJ+1) = SGFS(L)
  DE = 2.0 *DE
  DL = (ES(L)-ES(I))/DE

```

457


```

DO 45 N1=2,KJ
ET(N1) = ET(N1-1)+DL
INCJ = 1
SRENI = SQRT(ET(N1))
ST(N1) = C.O
SAT(N1) = C.C
SFT(N1) = C.C
DO 45 IN=1,NI
JIG = C
SGSP = C.C
SGAP = C.C
SGFP = C.C
DEL = -2.1566175E9 * R(IN) * SRENI
WL = 4.551E31E-10/SRENI
VAL2 = SIN(DEL)
EX1 = CMPLX(C.,-DEL)
CEXP1 = CEXP(EX1)
T2 = CEXP1 * VAL2 * WL
ABT2 = CABS(T2)
SGRI = C.O
JI = INCJ + NGI(IN) - 1
DO 46 IJ= INCJ,JI
SGAPR = C.C
SGFPR = C.O
JIG = JIG + 1
NRES = NR(IJ)
T1 = C.C
DO 47 N2=1,NRES
P1 = ET(N1) - EO(IJ,N2)
P2 = (GMN(IJ,N2) + GMG(IJ,N2) + GMF(IJ,N2))/2.O
DEN = CMPLX(P1,P2)
DENSP = P1**2 + P2**2
BLAMR = WL * SRENI/SQRT(ABS(EO(IJ,N2)))
SPCF = WL * BLAMR * GMN(IJ,N2)/DENSP
SGAPR = GMG(IJ,N2) * SPCF + SGAPR
SGFPR = GMF(IJ,N2) * SPCF + SGFPR
47 T1 = (GMN(IJ,N2)/2./DEN)*BLAMR + T1
VAL3 = T1 - T2
VAL1 = CABS(VAL3)
SGAP = SGAP + SGAPR * G(IN,JIG)
SGFP = SGFP + SGFPR * G(IN,JIG)
SGSP = SGAP + SGFP
48 SGRI = G(IN,JIG) * (VAL1**2 - ABT2**2) + SGRI
INCJ = INCJ + 2
ST(N1) = COEF(IN)*(SGRI+PSTM(IN)*ABT2**2+SGSP/4.O) + ST(N1)
SAT(N1) = COEF(IN)/4.O * SGAP + SAT(N1)
45 SFT(N1) = COEF(IN)/4.C * SGFP + SFT(N1)
DO 48 N1 = 2,KJ
LL = N1 + 1
IL = N1 - 1
IF(INTYP) 64,65,64
64 SK = ((ST(LL)-ST(IL))/(ET(LL)-ET(IL)))*(ET(N1)-ET(IL)) + ST(IL)
GO TO 66
65 RATIO = (ET(LL) - ET(N1))/(ET(LL) - ET(IL))
SK = ST(LL) * (ST(IL)/ST(LL))**RATIO
66 PK = (ABS(SK-ST(N1)))/ST(N1)*100.O
IF(PK.GT.DP) GO TO 41
48 CONTINUE
44 KC = KC + KJ-2
KJ = KJ + 1
KQ = NK + KJ
IF(KQ.GT.501) GO TO 49

```

OUTPUT STORAGE ON INTERMEDIATE POINTS

```

50 DO 51 N1= 2,KJ
NK = NK + 1
ER(NK) = ET(N1)
SGSR(NK) = ST(N1)-SAT(N1)-SFT(N1)
IF(SGSR(NK)) 67,67,68

```

C
C
C
C
C

```

67 SGSR(NK) = 0.C1
   SGTR(NK) = SAT(N1) + SFT(N1) + 0.01
   GO TO 69
68 SGTR(NK) = ST(N1)
69 SGAR(NK) = SAT(N1)
   ECIF = ER(NK) - ER(NK-1)
   FLGER = ALOG(ER(NK)/ER(NK-1))
   ADRAI(NK) = (SGAR(NK)-SGAR(NK-1))/EDIF*(EDIF-ER(NK-1)*FLGER)
   1 + SGAR(NK-1)*FLGER+ ADRAI(NK-1)
51 SGFR(NK) = SFT(N1)
   KM = 1
   GO TO 26

```

601

C
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C

COUNTER ON ELIMINATED PCINTS

```
36 KA = KA + KM
```

C
C
C
C
C

COUNTER ON PERCENT DEVIATION

```
TN = TN + DX
M = L-1
```

C
C
C
C
C

IF CUTPUT ARRAY IS FULL, PRINT,RETAIN LAST PCINT, AND EMPTY

```

42 IF(NK.LE.501) GO TO 53
49 WRITE (6,109)
   WRITE(6,105) (ER(KAM), SGTR(KAM), SGSR(KAM), SGAR(KAM), SGFR(KAM),
   1 ADRAI(KAM), KAM = 2,NK)
   NKST = NKST + NK - 1
   IF(PCF.EQ.C.C) GO TO 52
   WRITE(6,112)(ER(KAM),SGTR(KAM),SGSR(KAM),SGAR(KAM),SGFR(KAM),
   1 KAM = 2,NK)
52 IF(ES(M).EQ.EMX) GO TO 77
   ER(1) = ER(NK)
   SGAR(1) = SGAR(NK)
   ADRAI(1) = ADRAI(NK)
   DO 54 NKS = 2,NK
   ER(NKS) = C.C
   SGTR(NKS) = C.C
   SGSR(NKS) = C.C
   SGAR(NKS) = C.C
54 SGFR(NKS) = C.C
   NK = 1

```

618

619

632

C
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C

RETURN TO INTERMEDIATE PCINT SEQUENCING

C
C
C
C
C

```
IF(KQ.CT.500) GO TO 50
```

C
C
C
C
C

REGULAR STORAGE OF RETAINED PCINTS

```
53 NK = NK + 1
   ER(NK) = ES(M)
```

C
C
C
C
C

CORRECTION FOR NEGATIVE SCATTERING CROSS SECTION ARISING FROM EXCESSIVE INTERFERENCE DUE TO INADEQUACY OF G FACTOR= 1/2 APPROXIMATION AT S WAVE DIP BELOW SMALL RESONANCE SPACED BY LARGE RESONANCE---RARE SITUATION OCCURRING ONLY WHEN SPIN STATES ARE UNKNOWN

C
C
C
C
C

```

C
  SGSR(NK) = SGS(M) - SGAS(M) - SGFS(M)
  IF(SGSR(NK)) 7C,7C,71
7C SGSR(NK) = 0.01
  SGTR(NK) = SGAS(M) + SGFS(M) + 0.01
  GO TO 72
71 SGTR(NK) = SGS(M)
72 SGAR(NK) = SGAS(M)
  EDIF = ER(NK) - ER(NK-1)
  FLGER = ALOG(ER(NK)/ER(NK-1))

C
C
C   ACCUMULATIVE DILLTE RESONANCE ABSORPTION INTEGRAL
C
  ADRAI(NK) = (SGAR(NK)-SGAR(NK-1))/EDIF*(EDIF-ER(NK-1)*FLGER)
  1 + SGAR(NK-1)*FLGER+ ADRAI(NK-1)
  SGFR(NK) = SGFS(M)
26 CONTINUE

C
C   COUNTERS ON KA, TN
C
  KO1 = KO1 + KA
  CKO2 = CKO2 + TN

C
C   LOOP ON P POINTS
C
  KS = K1 + 1
  KCM = KIC * 125
  IF(J.LT.KCM) GO TO 13
  KI = KCM
  GO TO 11
13 IF(KI.EQ.J) GO TO 14
  KI = J
  GO TO 11

C
C   LOOP ON RESONANCES
C
14 ND = MC + 1
  ICM = IC * 83
  IF(NDES.LT.ICM) GO TO 18
  MD = ICM
  GO TO 16
18 IF(MD.EQ.NDES) GO TO 76
  MD = NDES
  GO TO 16

C
C   FINAL OUTPUT
C
76 WRITE (6,109)
  WRITE(6,105) (ER(KAM), SGTR(KAM), SGSR(KAM), SGAR(KAM), SGFR(KAM),
1 ADRAI(KAM), KAM = 2,NK)
  NKST = NKST + NK - 1
  IF(PCF.EQ.C.0) GO TO 77
  WRITE(6,112)(ER(KAM),SGTR(KAM),SGSR(KAM),SGAR(KAM),SGFR(KAM),
1 KAM = 2,NK)
77 TN = CKO2
  KA = KO1
  NJ = NJ + 1

C
C   SUMMARY OF CALCULATION
C
  WRITE(6,106) N,NKST,FD,PD,NJ,KA,KC,ICU
  DN = FLOAT(KA)
  TN = TN/DN
  WRITE(6,108) TN

```

```

100 FORMAT(1H1)
101 FORMAT(2I1C,4F1C.5,3I5,F5.C)
102 FORMAT(2F1C.5,E11.5,I9,F1C.5)
103 FORMAT(F1C.5,I1C)
104 FORMAT(F1C.5,I1C,3F10.5)
105 FURMAT(1HC6F2C.5)
106 FORMAT(1HC2CX3HFORI5,2X11HRESONANCES,I6,2X54HENERGY PCINTS ARE REQ
UIRED FOR DEVIATIONS OF LESS THAN//20XF5.1,2X9HBARNS ANCF5.1,2X31H
2PERCENT AT INTERPOLATED POINTS.//20>14HCF THE INITIALI5,2X7HPOINTS
3,
4I5,2X18FWERE DISCARDED ANDI5,2X32HADDITIONAL PCINTS WERE INSERTED.
5//2CXI5,2X46HPCINTS WERE RETAINED AS MAX,MIN OR INFLECTION.////)
107 FORMAT(1HC2CX14HREGION BETWEENF10.5,2X6HEV ANDF10.5,2X48HEV CANNOT
1 BE FITTED WITH 256 INTERMEDIATE PCINTS//)
108 FORMAT(1HC//20X45HAVERAGE PERCENT DEVIATION OF DISCARDED PCINTS//4
15XF10.5)
109 FORMAT(1HC6X6HENERGY14X11HSIGMA TOTAL9X13HSIGMA SCATTER7X13HSIGMA
1CAPTURE7X13HSIGMA FISSION6X14HACC. I(DILUTE)//)
110 FORMAT(1HL11X8HMASS NU.3X8HPCT. AB.5X11HNUC. RADIUS3X7HG VALUESX11
1HRES. ENERGY2X7HGAMMA N5X7HGAMMA G5X7HGAMMA F//)
111 FORMAT(1HC1CXF6.1,6XF6.4,6X1PE12.6,3X0PF6.4,3X4F12.5/)
112 FORMAT(1H$,1P$E12.5)
113 FORMAT(1I,1X,14A5)
114 FORMAT(2X,14A5)
115 FORMAT(1HL11X34HLINEAR INTERPOLATION WILL BE USED.)
116 FORMAT(1HL11X43HSEMILOGARITHMIC INTERPOLATION WILL BE USED.)
RETURN
ENC

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NATURAL TUNGSTEN

ALL PARAMETERS, WITH THE EXCEPTIONS NOTED BELOW, ARE TAKEN FROM REFERENCE A-1, WHICH DOES NOT LIST THE LOW ENERGY DATA. THE REMAINING PARAMETERS WERE CHOSEN ON THE BASIS OF CONSISTENCY WITH THE MAIN SOURCE, MINIMUM EXPERIMENTAL UNCERTAINTY, AND BEST PARAMETERS FOR MATCHING MEASURED VALUES OF THERMAL CROSS SECTIONS AND DILUTE RESONANCE INTEGRALS.

W-180 PARAMETERS FROM REFERENCE A-2.

W-182(-32.555 eV) AND W-184(-95.578 eV) HAVE ARBITRARY ENERGIES OBTAINED USING THE AVERAGED REDUCED NEUTRON WIDTH AND ASSUMED CAPTURE WIDTH OF REFERENCE A-1 TO MAKE UP THE DIFFERENCE BETWEEN THE THERMAL CROSS SECTIONS OF REFERENCE A-3 AND THE VALUES CALCULATED FROM THE KNOWN PARAMETERS.

W-182(4.16 AND 21.09 eV) AND W-183(7.67 eV) FROM REFERENCE A-4.

W-183(27.08 eV) FROM REFERENCE A-5.

W-182(46.2, 47.8, AND 45.3 eV) FROM REFERENCE A-6.

W-183(G FACTOR = 1/2 RESONANCES) FROM REDUCED NEUTRON WIDTHS, CAPTURE WIDTHS, AND ENERGIES GIVEN IN REFERENCE A-1.

W-186(18.83 eV) PARAMETERS FROM REFERENCE A-7.

THERMAL (0.0253 eV) ABSORPTION CROSS SECTIONS (BARNS)

	CALCULATED	REF. A-3
W-180	3.5	---
W-182	20.76	20.7(0.5)
W-183	8.89	10.0(0.3)
W-184	1.71	1.7(0.1)
W-186	35.61	37.8(1.2)
NAT. W	---	18.3(0.5)

INFINITELY DILUTE RESONANCE INTEGRALS (BARNS) ABOVE 0.5 eV

	CALCULATED	REF. A-7
W-180	204	---
W-182	623	---
W-183	355	---
W-184	15.6	15(2)
W-186	457	440(20)

CALCULATED VALUES HAVE AN UPPER LIMIT OF 2200 eV

REFERENCES

- A-1 BLOCK, R.C., FOCKENBURY, R.W., RUSSELL, J.E., THE PARAMETERS OF THE NEUTRON RESONANCES IN W-182, W-183, W-184, AND W-186, CRNL-3924, 31-35, (MAY 1966) (SEE ALSO RPI-328-56).
- A-2 JUNG, F., BLOCK, R.C., SLAUGHTER, G.G., PARAMETERS OF NEUTRON RESONANCES IN W-180, CRNL-3924, P. 30, (MAY 1966).
- A-3 FRIESENAHN, S.J., HADDAD, E., FRCHNER, F.H., LOPEZ, W.M., THE NEUTRON CAPTURE CROSS SECTION OF THE TUNGSTEN ISOTOPES FROM 0.01 TO 10 ELECTRON VOLTS, NUCLEAR SCIENCE AND ENGINEERING 26, 487-495 (1966).
- A-4 HARVEY, J.A., THE MEASUREMENT OF TOTAL NEUTRON CROSS SECTIONS IN THE RESONANCE ENERGY REGION AND THE DETERMINATION OF RADIATION WIDTHS OF RESONANCES, ANS TOPICAL MEETING ON REACTOR PHYSICS IN THE RESONANCE AND THERMAL REGION, P 10, SAN DIEGO (FEBRUARY 1966).
- A-5 PAYA, C., PEARCE, K.D., HARVEY, J.A., SLAUGHTER, G.G., PARAMETERS OF LOW ENERGY RESONANCES IN TUNGSTEN, CRNL-3582, 58-60 (JUNE 1964).
- A-6 RUSSELL, J.E., FOCKENBURY, R.W., BLOCK, R.C., NEUTRON CAPTURE MEASUREMENTS ON THE ISOTOPES OF TUNGSTEN, WASH-1046, P. 104 (JANUARY 1964).
- A-7 PEARCE, C.R., SHOOK, D.F., DETERMINATION OF TUNGSTEN RESONANCE ABSORPTION INTEGRALS BY ACTIVATION, NASA TN D- , (1967).

LINEAR INTERPOLATION WILL BE USED.

MASS NO.	PCT. AB.	NUC. RADIUS	G VALUE	RES. ENERGY	GAMMA N	GAMMA G	GAMMA F
14C.C	C.0013	8.470500E-13	1.0000	15.90000	0.C125C	C.C60C0	-0.
14O.C	C.C013	8.470500E-13	1.0000	49.30000	0.C062C	0.C60C0	-0.
14C.C	C.C013	8.470500E-13	1.0000	62.70000	0.C0140	0.C60C0	-0.
14C.C	0.0013	8.470500E-13	1.0000	75.20000	0.035C0	0.C60C0	-0.
14C.C	C.0013	8.470500E-13	1.0000	87.40000	0.CC73C	0.C60C0	-0.

MASS NO.	PCT. AB.	NUC. RADIUS	G VALUE	RES. ENERGY	GAMMA N	GAMMA G	GAMMA F
142.C	C.2631	8.500590E-13	1.0000	-32.99900	0.10514	C.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	4.16000	0.00148	0.C5400	-0.
142.C	C.2631	8.500590E-13	1.0000	21.09000	0.C433C	0.C62C0	-0.
142.C	C.2631	8.500590E-13	1.0000	98.00000	0.000C1	C.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	114.70000	0.290C0	0.C65C0	-0.
142.C	C.2631	8.500590E-13	1.0000	130.50000	0.C0050	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	214.00000	0.00280	C.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	250.00000	1.100C0	C.C64C0	-0.
142.C	C.2631	8.500590E-13	1.0000	283.00000	0.C011C	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	303.00000	0.00015	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	343.00000	0.C0E4C	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	378.00000	0.130C0	0.C65C0	-0.
142.C	C.2631	8.500590E-13	1.0000	410.00000	0.C002C	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	430.00000	0.280C0	0.C55C0	-0.
142.C	C.2631	8.500590E-13	1.0000	486.00000	0.500C0	0.C45C0	-0.
142.C	C.2631	8.500590E-13	1.0000	580.00000	0.300C0	0.C57C0	-0.
142.C	C.2631	8.500590E-13	1.0000	616.00000	0.CC14C	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	658.00000	0.160C0	0.C59C0	-0.
142.C	C.2631	8.500590E-13	1.0000	673.00000	0.C006C	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	762.00000	0.069C0	0.C74C0	-0.
142.C	C.2631	8.500590E-13	1.0000	785.00000	0.C14C0	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	866.00000	0.C21C0	0.C70C0	-0.
142.C	C.2631	8.500590E-13	1.0000	922.00000	0.400C0	0.C78C0	-0.
142.C	C.2631	8.500590E-13	1.0000	951.00000	2.200C0	0.C77C0	-0.
142.C	C.2631	8.500590E-13	1.0000	1010.00000	0.450C0	0.C76C0	-0.
142.C	C.2631	8.500590E-13	1.0000	1100.00000	1.600C0	C.C69C0	-0.
142.C	0.2631	8.500590E-13	1.0000	1170.00000	0.480C0	0.C58C0	-0.

MASS NO.	PCT. AB.	NUC. RADIUS	G VALUE	RES. ENERGY	GAMMA N	GAMMA G	GAMMA F
143.C	C.1428	8.516120E-13	0.2500	47.80000	0.115C0	C.C76C0	-0.
143.C	C.1428	8.516120E-13	0.2500	144.60000	0.C95C0	C.C50C0	-0.
143.C	C.1428	8.516120E-13	0.2500	154.90000	0.410C0	0.C80C0	-0.
143.C	C.1428	8.516120E-13	0.7500	7.67000	0.00174	C.C79C0	-0.
143.C	C.1428	8.516120E-13	0.7500	27.08000	0.C433C	C.C75C0	-0.

1E3.0	0.142E	E.516120E-13	0.7500	46.20000	0.15400	0.06800	-0.
1E3.C	C.1428	E.516120E-13	0.7500	65.30000	0.00100	0.07500	-0.
1E3.0	C.1428	E.516120E-13	0.7500	101.30000	0.05000	0.05800	-0.
1E2.C	C.1428	E.516120E-13	0.7500	157.30000	0.06700	0.06000	-0.
1E2.C	C.1428	E.516120E-13	0.7500	174.30000	0.05300	0.05000	-0.
1E2.C	C.1428	E.516120E-13	0.7500	192.60000	0.03500	0.07000	-0.
1E3.0	C.1428	E.516120E-13	0.7500	259.00000	0.05000	0.10000	-0.
1E2.C	C.1428	E.516120E-13	0.7500	280.00000	0.21000	0.07300	-0.
1E2.C	C.1428	E.516120E-13	0.7500	297.00000	0.03900	0.05900	-0.
1E2.C	C.1428	E.516120E-13	0.7500	323.00000	0.08200	0.05000	-0.
1E2.C	0.1428	8.516120E-13	0.7500	349.00000	0.14000	0.05500	-0.
1E2.C	C.1428	E.516120E-13	0.7500	361.00000	0.02500	0.07000	-0.
1E2.C	C.1428	E.516120E-13	0.7500	379.00000	0.07400	0.07800	-0.

MASS NO. PCT. AB. NUC. RADIUS G VALUE RES. ENERGY GAMMA N GAMMA G GAMMA F

1E2.C	C.1428	E.516120E-13	0.5000	40.70000	0.00615	0.06000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	104.10000	0.00615	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	138.30000	0.00564	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	203.80000	0.00343	0.08000	-0.
1E2.C	0.1428	E.516120E-13	0.5000	220.80000	0.00535	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	228.00000	0.00151	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	236.00000	0.01643	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	241.00000	0.05278	0.08000	-0.
1E2.C	C.1428	8.516120E-13	0.5000	244.00000	0.00533	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	289.00000	0.00748	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	338.00000	0.02020	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	354.00000	0.00530	0.08000	-0.
1E2.C	C.1428	E.516120E-13	0.5000	392.00000	0.04750	0.08000	-0.

MASS NO. PCT. AB. NUC. RADIUS G VALUE RES. ENERGY GAMMA N GAMMA G GAMMA F

1E4.0	0.3064	8.531660E-13	1.0000	-99.97500	0.24650	0.07000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	102.10000	0.00330	0.07000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	184.70000	1.20000	0.07800	-0.
1E4.C	C.3064	8.531660E-13	1.0000	244.00000	0.00240	0.07000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	311.00000	0.07500	0.05100	-0.
1E4.C	C.3064	8.531660E-13	1.0000	424.00000	0.04200	0.06500	-0.
1E4.C	C.3064	8.531660E-13	1.0000	595.00000	0.00100	0.07000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	684.00000	0.08000	0.07800	-0.
1E4.0	C.3064	8.531660E-13	1.0000	705.00000	0.00660	0.07000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	787.00000	0.02600	0.07000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	802.00000	1.00000	0.07500	-0.
1E4.0	C.3064	8.531660E-13	1.0000	961.00000	1.00000	0.11000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	1000.00000	0.14000	0.05500	-0.
1E4.C	C.3064	8.531660E-13	1.0000	1090.00000	3.40000	0.05500	-0.

1E4.C	C.3C64	8.531660E-13	1.0000	1140.00000	0.34000	0.C6000	-0.
1E4.C	C.3064	8.531660E-13	1.0000	1270.00000	1.20000	0.C6300	-0.
1E4.C	C.3C64	8.531660E-13	1.0000	1340.00000	0.C0210	0.C7000	-0.
1E4.0	C.3C64	8.531660E-13	1.0000	1410.00000	2.70000	0.C7600	-0.
1E4.C	C.3C64	8.531660E-13	1.0000	1430.00000	0.25000	0.C7500	-0.
1E4.C	C.3C64	8.531660E-13	1.0000	1520.00000	1.30000	0.05800	-0.
1E4.0	C.3C64	8.531660E-13	1.0000	1560.00000	0.C6800	0.C7000	-0.
1E4.0	C.3064	8.531660E-13	1.0000	1660.00000	0.25000	0.C8000	-0.
1E4.0	C.3C64	8.531660E-13	1.0000	1800.00000	1.10000	0.C6500	-0.
1E4.C	C.3064	8.531660E-13	1.0000	1880.00000	0.C3000	0.C7000	-0.
1E4.C	C.3C64	8.531660E-13	1.0000	1930.00000	0.25000	0.C7500	-0.

MASS NO. PCT. AB. NLC. RADIUS G VALUE RES. ENERGY GAMMA N GAMMA G GAMMA F

1E6.C	C.2E64	8.562420E-13	1.0000	18.83000	0.31500	0.C4100	-0.
1E6.C	C.2864	8.562420E-13	1.0000	111.30000	0.00004	0.C7000	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	171.50000	0.C2700	0.C7500	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	197.60000	0.C0000	0.C7000	-0.
1E6.C	C.2864	8.562420E-13	1.0000	218.00000	0.53000	0.C6200	-0.
1E6.C	C.2864	8.562420E-13	1.0000	245.00000	0.00020	0.C7000	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	288.00000	0.C2600	0.C7000	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	407.00000	0.C7500	0.C6200	-0.
1E6.C	C.2864	8.562420E-13	1.0000	458.00000	0.C0000	0.C7000	-0.
1E6.C	C.2864	8.562420E-13	1.0000	512.00000	0.C6500	0.C4500	-0.
1E6.C	C.2864	8.562420E-13	1.0000	543.00000	0.50000	0.C6500	-0.
1E6.C	C.2864	8.562420E-13	1.0000	666.00000	0.75000	0.C8500	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	732.00000	2.10000	0.C9200	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	774.00000	0.00600	0.C7000	-0.
1E6.C	C.2864	8.562420E-13	1.0000	835.00000	0.C2000	0.C7000	-0.
1E6.C	C.2864	8.562420E-13	1.0000	858.00000	0.C0200	0.C7000	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	968.00000	1.10000	0.C7200	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	1080.00000	0.65000	0.C6100	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	1130.00000	0.45000	0.C6200	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	1190.00000	0.77000	0.C5500	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	1420.00000	0.25000	0.C5000	-0.
1E6.C	C.2864	8.562420E-13	1.0000	1510.00000	1.20000	0.C6800	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	1550.00000	0.C0400	0.C7000	-0.
1E6.C	C.2864	8.562420E-13	1.0000	1800.00000	0.10000	0.C6500	-0.
1E6.C	C.2864	8.562420E-13	1.0000	1940.00000	0.55000	0.C6000	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	2040.00000	0.40000	0.C6700	-0.
1E6.C	C.2E64	8.562420E-13	1.0000	2120.00000	0.11000	0.C6700	-0.

ENERGY	SIGMA TOTAL	SIGMA SCATTER	SIGMA CAPTURE	SIGMA FISSION	ACC. I (DILUTE)
0.C25255556	21.568665504	4.110808134	17.457857370	-0.	-0.000000000
0.042255747	17.644255930	4.109911680	13.534348245	-0.	8.050632238

0.C59295499	15.567874193	4.109017253	11.458856540	-C.	12.291931272
0.C76295243	14.234938622	4.108123541	10.126815081	-C.	15.019442558
C.C53295654	13.287731886	4.107230544	9.180501242	-C.	16.964428186
0.11C295745	12.57C75E462	4.106338263	8.464420159	-C.	18.442830801
0.1272956457	12.004122496	4.105446517	7.898675978	-C.	19.616559505
0.144295E241	11.542C16387	4.104555130	7.437461257	-C.	20.578337193
0.1612957992	11.156C45490	4.103664279	7.052385211	-C.	21.385611057
0.17E297743	1C.827566385	4.102773666	6.724792719	-C.	22.076130629
0.1992957455	10.543737650	4.101882994	6.441854E56	-C.	22.675863504
0.212297238	10.295413613	4.100992799	6.194420815	-C.	23.203340054
0.229295699C	10.075E6E607	4.100102782	5.975765E24	-C.	23.672186851
0.24E2956741	9.880C35400	4.099212706	5.780822654	-C.	24.092679501
0.2E32956452	9.704C12871	4.098322690	5.605690181	-C.	24.472733021
C.2E0295E23E	9.544743180	4.097432613	5.4473105E7	-C.	24.818557262
0.297295555	9.399791241	4.096542478	5.30324E7E3	-C.	25.135101795
0.E412E7953	7.53C248344	4.067599654	3.462648E6C	-C.	29.857317209
1.7932735E5	7.CC9766161	4.006211638	3.003554493	-C.	32.326045036
2.87563E0C8	8.14058C416	3.847042620	4.29353779E	-C.	34.025119781
3.2E6772C02	10.235449510	3.695003390	6.54044E52C	-C.	34.712892056
3.52752E01E	14.350287318	3.505337715	10.844949E03	-C.	35.378332615
3.6E79C599E	15.220681429	3.361116529	15.8595645C0	-C.	35.862383842
3.723C950C0	23.451154709	3.273392439	20.177762270	-C.	36.180564404
3.7E82E4CC4	3C.059C46469	3.178499460	26.920547C09	-C.	36.589158058
3.820878506	34.945631981	3.132136345	31.813495E2E	-C.	36.840725899
3.EE2473C0E	41.411273956	3.091688633	38.319585323	-C.	37.138567448
3.EE6C67510	5C.3C0E37C40	3.065764904	47.23507213E	-C.	37.498832703
3.91E6E2C12	62.9E5734463	3.071518421	59.91421E042	-C.	37.946254253
3.9249E92E3	71.459150314	3.096199989	68.362950325	-C.	38.212457657
3.9512E6514	81.955331802	3.144636154	78.81069564E	-C.	38.516617298
3.9E75E37E5	95.166656494	3.228197098	91.93845935E	-C.	38.868031502
3.9E38E1C1E	112.105991364	3.364455223	108.74153E14C	-C.	39.279355049
4.0CC14E237	134.30C188065	3.581350327	130.71883773E	-C.	39.768147945
4.01E445458	164.133132935	3.924852371	160.2082805E3	-C.	40.359637260
4.032742679	205.482116699	4.473558426	201.00855E273	-C.	41.091009617
4.C4504C02C	2E4.966739655	5.368614197	259.59812545E	-C.	42.019774437
4.0E9845C21	387.31264E773	7.466571808	379.846076965	-C.	43.658286571
4.CE232E022	5C5.205785461	9.702808380	495.506977C81	-C.	44.999054909
4.094811022	683.232276916	13.341011047	669.8912658E9	-C.	46.778362751
4.1C3133023	855.62C712280	17.078094482	838.542617758	-C.	48.309873104
4.1C7294023	965.13858C322	19.537063599	945.601516724	-C.	49.214548111
4.1114E5C23	1094.7E8676758	22.519088745	1072.249588C12	-C.	50.236818790
4.11561E024	1248.874603271	26.152420044	1222.7221E3228	-C.	51.398771286
4.115777024	1432.643478394	30.595443726	1402.048034E6E	-C.	52.727295876

4.123928024	1651.987335205	36.038360596	1615.948974605	-C.	54.251762390
4.128099024	1913.112152100	42.697601318	1870.414590781	-C.	56.013356209
4.123647025	2335.239166260	53.845367432	2281.393798828	-C.	58.804238796
4.127808025	2709.036495023	64.105133057	2644.931365567	-C.	61.287439823
4.146120025	3554.989532471	88.895812988	3466.093719482	-C.	67.426372528
4.190291026	3959.578582764	101.929351807	3857.649230957	-C.	71.102688789
4.193065026	4183.887207031	109.858734131	4074.028472900	-C.	73.755782127
4.195829026	4348.421691895	116.502502441	4231.919189452	-C.	76.531302452
4.197226026	4402.722595215	119.165344238	4283.557250977	-C.	77.952976227
4.198613026	4436.179592676	121.309265137	4314.870727539	-C.	79.388350487
4.190000026	4447.822814541	122.890380859	4324.932424082	-C.	80.829081535
4.191366567	4437.315002441	123.881103516	4313.433896926	-C.	82.268830299
4.192713967	4404.975952148	124.270751953	4280.705200195	-C.	83.699986458
4.195547967	4279.189086914	123.294677734	4155.894409180	-C.	86.509539604
4.198321967	4084.234405518	120.210144043	3964.024261475	-C.	89.210590363
4.172482967	3704.152313232	112.599822998	3591.552490234	-C.	92.974343300
4.178020968	3133.868286133	99.504547119	3034.363739014	-C.	97.375096321
4.183578968	2590.493133545	85.949829102	2504.543304443	-C.	101.045792580
4.187735968	2232.804016113	76.580963135	2156.223052979	-C.	103.358903885
4.191900969	1924.383300781	68.235794067	1856.147506714	-C.	105.349685669
4.196061969	1662.989227295	60.965011597	1602.024215698	-C.	107.064538956
4.200222969	1443.284759521	54.703170776	1388.581588745	-C.	108.546264648
4.204383969	1259.109466553	49.337020874	1209.772445679	-C.	109.832181931
4.208544970	1104.580322266	44.742370605	1059.837951660	-C.	110.953846931
4.212705970	974.528137207	40.801406880	933.726730347	-C.	111.937504768
4.221027970	771.211875916	34.479545593	736.732330222	-C.	113.585330009
4.225349971	622.543305969	29.715682983	593.227622986	-C.	114.895122528
4.241832972	467.632614136	24.538002014	443.094612122	-C.	116.421575546
4.246476972	335.900852203	19.931400299	315.969451904	-C.	117.907953262
4.270959973	270.356330872	17.531406403	252.824924469	-C.	118.740366936
4.236148973	115.664155960	11.337471962	104.326683998	-C.	121.448160172
4.401337922	65.653623581	8.989222527	56.664401054	-C.	122.650173187
4.433932424	52.680656910	8.311931133	44.368725777	-C.	123.022937775
4.466526926	43.565114975	7.807105064	35.758009911	-C.	123.316404343
4.499121428	36.918286324	7.418309927	29.499976397	-C.	123.553673744
4.531715930	31.923838854	7.110941410	24.812897444	-C.	123.749719620
4.662093937	20.659891129	6.344658494	14.315232635	-C.	124.305338860
4.857660949	14.041173935	5.810591578	8.230582356	-C.	124.769424438
5.183609969	10.271516747	5.451491058	4.820425689	-C.	125.194414139
5.800869048	8.519005775	5.284209371	3.234796405	-C.	125.649219513
6.085477531	8.394903302	5.288650870	3.106252422	-C.	125.801103592
6.844433486	9.601751924	5.391392946	4.210358977	-C.	126.229794502
7.129041970	12.103486419	5.425990999	6.677495420	-C.	126.451245308
7.223911464	14.139810681	5.430888414	8.708922267	-C.	126.552917480

7.271346211	15.733036160	5.432405829	10.300630331	-C.	126.615120888
7.318760959	18.000871897	5.434687614	12.566184262	-C.	126.689459801
7.366215706	21.385763884	5.440934181	15.944825702	-C.	126.781545639
7.413650453	26.756425951	5.459326029	21.299095922	-C.	126.901064873
7.514575461	57.415153027	5.701188564	51.713964462	-C.	127.394231796
7.550908446	88.815578461	6.077634811	82.737943649	-C.	127.718454361
7.561185937	142.591823578	6.869661331	135.722162247	-C.	128.155666351
7.605407953	229.236886978	8.365262985	220.871623993	-C.	128.724721909
7.623574436	347.655506677	10.682868958	336.973037720	-C.	129.390148163
7.641740978	538.311599731	14.927673340	523.383926392	-C.	130.414619446
7.649814963	640.617500305	17.499565125	623.117925161	-C.	131.021064758
7.661925972	769.265159607	21.364532471	747.900627136	-0.	132.105680466
7.670000017	800.368080139	23.048080444	777.319999695	-0.	132.909090042
7.676074002	770.536581848	23.420906067	747.117675761	-C.	133.710794449
7.692203462	617.803199768	21.351158142	596.452041626	-C.	134.945844650
7.694221573	552.154174805	20.899909973	571.254264832	-C.	135.098976135
7.710370004	405.676821899	17.213455200	388.763366699	-C.	136.104303360
7.728536487	265.139163971	14.023357391	251.115806580	-C.	136.856510162
7.752756443	161.656569290	11.431249619	150.425319672	-C.	137.484615326
7.783035934	98.973272324	9.691202164	89.282070160	-C.	137.951662064
7.819366956	63.102967739	8.601566315	54.501401424	-C.	138.286458969
7.831479967	55.730446815	8.363546371	47.366900444	-C.	138.365261078
7.855197310	44.995426178	8.004860401	36.990565777	-C.	138.492776871
7.878914654	37.523616791	7.744807005	29.778809766	-C.	138.593425751
7.902631996	32.127161980	7.550552368	24.576609612	-C.	138.675113678
7.926345342	28.109384298	7.402010202	20.707374056	-0.	138.742950439
7.950066666	25.041463375	7.286328793	17.755134563	-C.	138.800407410
7.973764029	22.646416042	7.194965124	15.453450516	-C.	138.849868774
7.997901373	20.747639656	7.122049689	13.625589967	-C.	138.893045425
8.021218856	19.214159012	7.063432097	12.150726914	-C.	138.931209564
8.116088390	15.323706665	6.922232032	8.401474833	-C.	139.052074432
8.305827379	12.158560514	6.857441485	5.301119030	-C.	139.210536957
8.760174851	10.456808090	7.092889428	3.363918622	-C.	139.451656342
8.96913840	10.399690151	7.254678786	3.145011336	-C.	139.521244049
10.593345661	12.891876578	9.690242171	3.201634316	-C.	140.048994064
12.322297931	20.011977911	15.569681168	4.442296743	-C.	140.624452591
13.619011879	31.758782625	25.375525236	6.383257210	-C.	141.164415359
14.647562365	50.979854107	41.632131577	9.347722520	-C.	141.735769272
15.499437332	83.721459389	69.468955040	14.252503753	-C.	142.401521683
15.631124783	112.299795151	88.873520851	23.426274300	-C.	142.800090790
15.690937328	143.081237793	97.462361336	45.618875960	-C.	142.930261612
15.901812434	146.121927261	98.715823174	47.406104068	-0.	142.962102890
15.934437354	132.057069778	98.347208023	33.709861755	-C.	143.045139313
15.990624905	122.898665428	100.063799858	22.834865332	-C.	143.144659042

16.452416382	178.71875C000	151.763008118	26.955740650	-C.	143.913547516
16.5742456C1	25C.959415436	249.589328766	41.3700E5235	-C.	144.896333694
17.2E3595681	425.526296234	367.597076416	58.3292183EE	-C.	145.797342300
17.45C459725	572.63037E723	496.161808014	76.4685688C2	-C.	146.597604752
17.6425E3113	758.4C6555176	659.242706299	99.16384EE77	-C.	147.457208633
17.7E5E23135	914.821E15491	796.712173462	118.1096363C7	-C.	148.090398788
17.EE50E31EE	1122.873321533	979.727584839	143.145726654	-C.	148.847354889
17.95791E517	1301.567193604	1137.384201050	164.5829E8735	-C.	149.438930511
18.CC6745E6E	1525.7C2667236	1334.453704834	191.248956E8C	-C.	150.120365143
18.0755E322C	1805.793594360	1584.829635620	224.96394725E	-C.	150.914340973
18.136595E45	2132.767639160	1869.627593994	263.14004516E	-C.	151.742181778
18.15C95974E	2490.279571533	2185.030517578	305.249027252	-C.	152.587135315
18.217959657	27C2.114196777	2371.975585937	330.1385955E1	-C.	153.058361053
18.244959647	2940.828887939	2582.689117432	358.139751434	-C.	153.568162918
18.271595E36	321C.970153809	2821.195739746	389.7743873E0	-C.	154.121232986
1E.2589597E6	351E.C25418945	3092.357147217	425.67226C2E4	-C.	154.723484039
18.325959727	3868.65046C205	3402.091583252	466.59885025C	-C.	155.381383896
18.3525956E7	4271.116577148	3757.628692627	513.487876892	-C.	156.103029251
1E.375959638	4735.325622559	4167.841796875	567.4837799C7	-C.	156.898090363
1E.4C6595E26	5273.666E25977	4643.671203613	629.9954223E3	-C.	157.777486801
18.4E3395977	59C1.388E5498C	5198.629089355	702.75975C3E6	-C.	158.754465103
18.46C595727	EE37.3E7878418	5849.462524414	787.92533111E	-C.	159.845474243
18.4E795967E	75C5.C30822754	6616.886474609	888.14430595E	-C.	161.070623398
18.51495962E	8533.0E6C59570	7526.411987305	1006.674041748	-C.	162.453268051
18.541959817	9756.593C17578	8609.121826172	1147.471176147	-C.	164.022789001
18.5EE9597E7	11217.25655E0C8	9902.029052734	1315.227890015	-C.	165.815568924
1E.559595718	129E2.754795805	11447.509643555	1515.28509521E	-C.	167.872980118
1E.622959668	15043.536376553	13290.308349609	1753.227920522	-C.	170.246139526
18.649959E57	17503.840087891	15469.953125000	2033.886871238	-C.	172.990770340
1E.65E9596E1	18412.958779297	16275.582031250	2137.41665E454	-C.	173.998075485
18.6E7959744	19366.775634766	17120.853271484	2245.922149E5E	-C.	175.056886673
1E.67E595E8C7	203E4.C27C99E09	18004.770019531	2359.257080C7E	-C.	176.170106888
18.6EE959E7C	21402.585843750	18925.431640625	2477.1581726C7	-C.	177.336496353
1E.6E4959E95	22479.0C7324219	19879.793701172	2599.21359252E	-C.	178.562240601
18.7C395975E	23588.414794E22	20863.564453125	2724.850219727	-C.	179.844430923
18.721959E8E4	25E77.522705C78	22893.997070312	2983.52557273C	-C.	182.591482162
18.73C9597C8	27037.84887E953	23923.527587891	3114.321075425	-C.	184.059986114
1E.735959771	28152.156777344	24948.007568359	3244.1892089E4	-C.	185.587839127
18.74E959834	29325.350585937	25953.965820312	3371.3847351C7	-C.	187.178663254
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19.144955504	8547.108276367	7954.488098145	992.620162964	-C.	243.893074036
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27.118447304	2733.355072021	1033.961044312	1699.394027710	-C.	335.337635040
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27.281109810	345.475067139	155.680753708	193.794313431	-C.	339.063842773
27.316599846	268.565544128	124.934301376	143.631242752	-C.	339.283172607
27.400769711	166.891721725	85.819760323	81.071961403	-C.	339.628677368
27.484929814	119.265115553	67.120431900	52.144687653	-C.	339.832988739
27.569109678	93.153319359	56.635271549	36.518047810	-C.	339.968540192
27.737449646	66.732913017	45.641374588	21.091538429	-C.	340.143898010
27.969999717	49.964362144	38.152446747	11.811915159	-C.	340.293037415
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30.000000000	26.717815399	24.564364195	2.153451204	-C.	340.651081085

FOR 115 RESONANCES, 345 ENERGY POINTS ARE REQUIRED FOR DEVIATIONS OF LESS THAN 10.0 BARNS AND 5.0 PERCENT AT INTERPOLATED POINTS.

OF THE INITIAL 861 POINTS, 548 WERE DISCARDED AND 32 ADDITIONAL POINTS WERE INSERTED. 19 POINTS WERE RETAINED AS MAX, MIN OR INFLECTION.

AVERAGE PERCENT DEVIATION OF DISCARDED POINTS

1.97583

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