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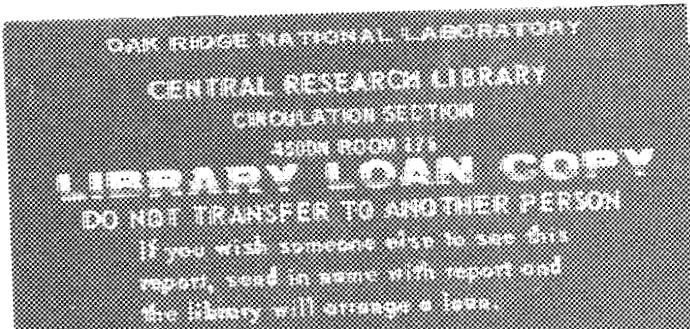
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URR Computer Code: A Code to
Calculate Resonance Neutron
Cross-Section Probability Tables,
Bondarenko Self-Shielding Factors,
and Self-Indication Ratios for
Fissile and Fertile Nuclides

L. C. Leal
G. de Saussure
R. B. Perez



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Engineering Physics and Mathematics

**URR Computer Code: A Code to Calculate
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Tables, Bondarenko Self-Shielding Factors, and
Self-Indication Ratios for Fissile and Fertile Nuclides**

L. C. Leal, G. de Saussure, and R. B. Perez

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ABSTRACT

The URR computer code has been developed to calculate cross-section probability tables, Bondarenko self-shielding factors, and self-indication ratios for fertile and fissile isotopes in the unresolved resonance region. Monte Carlo methods are utilized to select appropriate resonance parameters and to compute the cross sections at the desired reference energy.

The neutron cross sections are calculated by the single-level Breit-Wigner formalism with s -, p -, and d -wave contributions. The cross-section probability tables are constructed by sampling the Doppler broadened cross-section.

The various shelf-shielded factors are computed numerically as Lebesgue integrals over the cross-section probability tables.

1. INTRODUCTION

The URR (Unresolved Resonance Region) computer code was developed to study the effect of various assumptions on the statistical distributions of unresolved resonance parameters on self-shielding factors and self-indication ratios. The code uses the Monte Carlo method to compute cross-section probability tables. It then utilizes these tables to compute Bondarenko self-shielding factors and self-indication ratios. Consistent with ENDF/B procedures for the unresolved resonance region, all calculations are done in the single-level Breit-Wigner approximation. The code generates directly the cross-section probability tables at a user-specified energy and temperature from user-provided unresolved resonances parameters; the code does not sample from consecutive points on a statistical ladder, as most other codes of this type do,^{1,4} and extend the calculations of self-shielding factors and self-indication ratios for fissile nuclides.

These new features led to an improvement in the efficiency and reliability in the calculation of reactor parameters in the unresolved resonance region.

The code was developed and implemented on a VAX-11/785 computer.

This report describes the program and is also intended to serve as a user guide.

2. CROSS-SECTION FORMULA

The single-level Breit-Wigner formula for the unbroadened capture, fission and total cross sections are given in Table 1. For each series (L, J) (L -neutron orbital angular momentum, J -total angular momentum) contributing to the cross sections, the user must specify the values of L , and $G(L, J)$ (spin statistical factor), the average values of $D(L, J)$ (average level spacing), $GN(L, J)$ (average neutron reduced width), $GC(L, J)$ (gamma width), $FW(L, J)$ (average fission width) and the number of degrees of freedom, $NUM(L, J)$ and $NUF(L, J)$ of the chi-squared distribution laws for $GN(L, J)$ and $FW(L, J)$ respectively. The radiation widths GC are assumed to be constant for a given (L, J) -pair; the nearest neighbor level spacing for a (L, J) -series are assumed to follow a Wigner distribution with average value $D(L, J)$. Correlations of successive spacings implied by the Dyson-Metha Δ_3 -statistics² are ignored. Only values of $L = 1, 2$ or 3 are assumed to contribute; higher angular-momentum contributions are normally negligible in the resonance region.

Table 1. Unbroadened Cross Section

a. Capture and Fission Cross Section

$$\sigma_{n,c}^\ell = \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{NRJ} \frac{\Gamma_{nr}\Gamma_{cr}}{(E - E_r)^2 + \frac{\Gamma_r^2}{4}}$$

where c can be capture γ , or fission f .

b. Total Cross Section

$$\begin{aligned} \sigma_{n,t}^\ell &= \sigma_{pot} + \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{NRJ} \frac{\Gamma_{nr} [\Gamma_r \cos 2\varphi_\ell + 2(E - E_r) \sin 2\varphi_\ell]}{(E - E_r)^2 + \frac{\Gamma_r^2}{4}} \\ \sigma_{pot} &= \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \varphi_\ell \end{aligned}$$

The symbols have the usual meaning as defined, for instance, in reference 6.

The user must also provide values for the ratio of the mass of nucleus considered to the neutron mass $AWRI$, and for scattering radius AP . These values are used to

compute the potential scattering cross section and the shift and penetration factors. The user also specify IPAIRS, the number of pairs of resonances which contribute to the cross sections at the reference energy. An equal number of resonances is included below and above the reference energy.

The Doppler broadening of the cross sections is approximated by averaging the unbroadened cross sections over a Maxwellian distribution of velocities. The formalism utilized is the same as that described in MC-2.³ The formulae for the Doppler-broadened cross sections are given in Table 2.

Table 2. Broadened Cross Section

a. Capture and fission cross section

$$\sigma_{n,c} = \frac{2\pi^{3/2}}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}^{(\ell,J)} \Gamma_{cr}^{(\ell,J)}}{\Gamma_r^{(\ell,J)}} \frac{U(x,y)}{\Delta}$$

where c can be capture γ , or fission f .

b. Total cross section

$$\sigma_T^\ell = \sigma_{pot} + \frac{2\pi^{3/2}}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \Gamma_{nr}^{(\ell,J)} \left(\frac{U(x,y)}{\Delta} \cos 2\varphi_\ell - \frac{V(x,y)}{\Delta} \sin 2\varphi_\ell \right)$$

where $U(x,y)$ and $V(x,y)$ are related to the Voight profiles ψ, χ function, as
 $\psi(x,\theta) = \sqrt{\pi}bU(a,b)$
 $\chi(x,\theta) = \sqrt{\pi}bV(a,b)$

And Δ is the Doppler width.

3. SAMPLING PROCEDURE

For each (L, J) -series of resonances contributing to the cross sections the spacing surrounding the reference energy is selected from the probability distribution

$$P(x)dx = xW(x)dx , \quad (1)$$

where $W(x)dx$ is the Wigner spacing distribution:

$$W(x)dx = (\pi/2)x \exp(-(\pi/4)x^2)dx , \quad (2)$$

where $x = D / < D >$ and $< D >$ is the mean spacing $D(L, J)$ of the level series.

The position of the reference energy in the surrounding spacing is selected from a uniform distribution:

$$P(x)dx = dx/s , \quad (3)$$

where s is the width of the spacing.

The reduced neutron widths and fission widths of all the resonances considered are selected from the specified chi-squared distribution. The level spacing, except for the central level spacing discussed above, are selected from a Wigner distribution (Eq. 2).

For each history, the total fission and capture cross sections at the reference energy are obtained by summing the contribution of all the resonance considered.

4. CROSS-SECTION PROBABILITY TABLE

The total capture and fission cross sections at the reference energy are computed with each iteration. The probability distribution for the total cross section is parsed on a table. The number of entries and widths of the probability table can be specified by the users. If no specification is given a default recommended by Otter⁴ is used. With the probability PTK of the total cross section falling in the k^{th} interval of the table, the average values of the fission and capture cross sections corresponding to that entry are also stored. The standard deviation of the probability PTK is computed from

$$\sigma = (PTK * (1 - PTK)/NL)^{1/2} \quad (4)$$

where NL is the number of iterations.

5. TRANSMISSION AND SELF-INDICATION SELF-SHIELDING RATIOS

Average transmission, average capture, and average fission self-indication factors for a given thickness n are computed according to the expressions,

$$T(n) = \sum_{k=1}^{NL} \frac{PT(k)}{NL} \exp\left(-n \frac{\sigma_T(k)}{PT(k)}\right) \quad (5)$$

$$S_c(n) = \frac{\sum_{k=1}^{NL} \sigma_c(k) \exp\left(-n \frac{\sigma_T(k)}{PT(k)}\right)}{\sum_{k=1}^{NL} \sigma_c(k)} \quad (6)$$

$$S_f(n) = \frac{\sum_{k=1}^{NL} \sigma_f(k) \exp\left(-n \frac{\sigma_T(k)}{PT(k)}\right)}{\sum_{k=1}^{NL} \sigma_f(k)} \quad (7)$$

6. SELF-SHIELDED CROSS SECTIONS

The self-shielded cross sections are computed for each dilution specified using the Bondarenko⁵ formalism.

The expression for the self-shielded capture, fission, and total diluted cross section for a dilution σ_o is,

$$\sigma_c(\sigma_o) = \frac{\sum_{k=1}^{NL} \frac{\sigma_c(k)}{\left(\frac{\sigma_T(k)}{PT(k)}\right) + \sigma_o}}{\sum_{k=1}^{NL} \frac{PT(k)}{\left(\frac{\sigma_T(k)}{PT(k)}\right) + \sigma_o}} \quad (8)$$

$$\sigma_f(\sigma_o) = \frac{\sum_{k=1}^{NL} \frac{\sigma_f(k_0)}{\left(\frac{\sigma_T(k)}{PT(k)}\right) + \sigma_o}}{\sum_{k=1}^{NL} \frac{PT(k)}{\left(\frac{\sigma_T(k)}{PT(k)}\right) + \sigma_o}} \quad (9)$$

$$\sigma_T(\sigma_o) = \frac{\sum_{k=1}^{NL} \frac{PT(k)}{\left(\frac{\sigma_T(k)}{PT(k)}\right) + \sigma_o}}{\sum_{k=1}^{NL} \frac{PT(k)}{\left(\frac{\sigma_T(k)}{PT(k)} + \sigma_o\right)^2}} - \sigma_o \quad (10)$$

7. REFERENCES

1. J. G. Munoz-Cobos, *PAPIN: A Fortran-IV Program to Calculate Cross Section Probability Tables, Bondarenko and Transmission Self-Shielding Factors For Fertile Isotopes in the Unresolved Resonance Region*, Oak Ridge National Laboratory, ORNL/TM-7883 (August 1981).
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4. J. M. Otter et al., *U3R: A Code to Calculate Unresolved Resonance Cross Section Probability Tables*, Atomic International, AI-AEC-13024(1972).
5. I. I. Bondarenko et al., *Group Constant for Nuclear Reactor Calculations*, Consultant Bureau, New York (1964).
6. Data Format and Procedures for the Evaluated Nuclear Data File, ENDF, revised by R. Kinsey, BNL-NCS-50496 (ENDF-102), Second edition (ENDF/B-V), UC-80 (General Technology-TID-4500).

8. INPUT DESCRIPTION

All variables are entered to the code in free format. In each entry the variables are separated by commas.

The structure of the input is as follows:

1. ACCEPT 100, AW, AWRI, AP, EREF, TEMP, NL, IPAIRS, SEED

where:

AW – Mass number of the isotope.
AWRI – Ratio of the mass of the target nucleus to neutron mass.
AP – Scattering radius in units of 1.0E-12 cm.
EREF – Resonance energy (in eV).
TEMP – Temperature in K units.
NL – Number of iterations.
IPAIRS – Number of pairs of resonance levels which contribute to the cross section at the energy EREF.
SEED – Initial seed for the random number generator

2. ACCEPT 101, L, G, D, G0, GC, FW, NUM, NUF

where:

L – Neutron orbital angular momentum.
G – Spin statistical factor.
D – Average level spacing for resonances with total spin J (in eV)
G0 – Average reduced neutron width (in eV).
GC – Average radiation width (in eV).
FW – Average fission width (in eV).
NUM – Number of degrees of freedom in the neutron width distribution.
NUF – Number of degrees of freedom in the fission width distribution.

Note: Several series of resonance parameters can be given. The last card must be a blank card.

3. ACCEPT 102, CST3, CSC3, CSF3

where:

CST3, CSC3, CSF3 – FILE 3 contribution (in barns) to the total, capture and fission cross sections.

4. ACCEPT 103, NPT, CSMIN, CSMAX

where:

NPT – Number of entries for the construction of the probability table.
CSMIN – Lower limit of the band structure.
CSMAX – Upper limit of the band structure.

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Note: For default type a blank card.

5. ACCEPT 104, (SIGDIL(M), M = 1, 10)

where:

SIGDIL(M) - Values of the thicknesses (atoms/barn) for the calculation of the self-indication and transmission ratios. Up to ten consecutive values are allowed. If the number of thicknesses are less than ten, the last value must be zero.

6. ACCEPT 104, (SIGDIL(M), M = 1, 10)

where:

SIGDIL(M) - Values of the dilution cross section (barn) for the calculation of the Bondarenko partial and transport cross section. Up to ten consecutive values are allowed. If the number of dilution are less than ten, the last value must be zero.

9. OUTPUT DESCRIPTION

Unless otherwise specified by the user the output of URR is contained in a file called OUTPUT.URR. This file contains the value of the probability table as well as the cross-section probability table for the number of entries specified by the input variable NPT. Also the average cross-section self-shielding cross section, transmission, and self-indication ratios are given as output. In Appendix B a sample case is given to illustrate the output of the code.

APPENDIX A. FORTRAN LISTING OF URR

```
***** URR COMPUTER CODE *****
*
*
*
* INPUT DESCRIPTIONS
*
* 1. ACCEPT 100, AW, AWRI, AP, EREF, TEMP, NL, IPAIRS, SEED
* Where:
* AW - Mass number of the isotope.
* AWRI - Ratio of the mass of the target nucleus to neutron mass.
* AP - Scattering radius in units of 1.0E-12 cm.
* EREF - Resonance energy (in eV).
* TEMP - Temperature in K units.
* NL - Number of iterations.
* IPAIRS - Number of pairs of resonance levels which contribute to the
* cross section at the energy EREF.
* SEED - Initial seed for the random number generator.
*
* 2. ACCEPT 101, L, G, D, GO, GC, FW, NUM, NUF
* Where:
* L - Neutron orbital angular momentum.
* G - Spin statistical factor.
* D - Average level spacing for resonances with total spin J (in eV)
* GO - Average reduced neutron width (in eV).
* GC - Average radiation width (in eV).
* FW - Average fission width (in eV).
* NUM - Number of degrees of freedom in the neutron width distribution.
* NUF - Number of degrees of freedom in the fission width distribution.
* Note: Several series of resonance can be given. The last card must be
* a blank card.
*
* 3. ACCEPT 102, CST3, CSC3, CSF3
* Where:
* CST3, CSC3, CSF3 - FILE 3 contribution (in barns) to the total,
* capture and fission cross sections.
```

```

*
* 4. ACCEPT 103, NPT, CSMIN, CSMAK
*
* Where:
*
* NPT - Number of entries for the construction of the probability table.
*
* CSMIN - Lower limit of the band structure.
*
* CSMAK - Upper limit of the band structure.
*
* Note: For default type a blank card.
*
* 5. ACCEPT 104, ( SIGDIL(M), M = 1, 10 )
*
* Where:
*
* SIGDIL(M) - Values of the thicknesses (atoms/barn) for the calculation
* of the self-indication and transmission ratios. Up to ten
* consecutive values are allowed. If the number of thicknesses
* are less than ten, the last value must be zero.
*
* 6. ACCEPT 104, ( SIGDIL(M), M = 1, 10 )
*
* Where:
*
* SIGDIL(M) - Values of the dilution cross section (barn) for the
* calculation of the Bondarenko partial and transport cross
* section. Up to ten consecutive values are allowed. If the
* number of dilution are less than ten, the last value must be
* zero.
*****
CHARACTER*30 FIN
DIMENSION V(3),SIN2FI(3),COS2FI(3)
DIMENSION LS(6),GS(6),DS(6),GN(6),GG(6),GF(6),NN(6),NF(6)
DIMENSION PT(50),CSTK(50),CSCK(50),CSFK(50)
DIMENSION XI(20)
DIMENSION SIGDIL(10)
INTEGER*4 SEED
COMMON SEED
TYPE *, 'Output file name. (Default is OUTPUT.URR) '
ACCEPT '(A)', FIN
OPEN(UNIT=1, FILE = FIN, STATUS = 'NEW',
* DEFAULTFILE = 'OUTPUT.URR')
SIGN = 1.0
AKO = 0.002196771
FOURPI = 12.56637
ROOTPI = 1.772454
CTP = 1.128379
AKB = 3.44672E-4
C
TYPE *, 'TYPE AW, AWRI, AP, EREF, TEMP, NL, IPAIRS,
* SEED'
ACCEPT 100, AW, AWRI, AP, EREF, TEMP, NL, IPAIRS, SEED
C
IF( IPAIRS .EQ .0 ) IPAIRS = 1
C
WRITE(1, 1000)
WRITE(1, 1001) AW, AWRI, AP, EREF, TEMP, NL, IPAIRS
C
RTEREF = SQRT(EREF)

```

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```

AK = AK0 * RTEREF * AWRI / (AWRI + 1.0)
A = 0.123 * AWRI**0.333333 + 0.08
RHO = AK*A
RHOSQ = RHO * RHO
RHO4 = RHOSQ * RHOSQ
V(1) = 1.0
V(2) = RHOSQ / (1.0 + RHOSQ)
V(3) = RHO4 / (9.0 + 3.0 * RHOSQ + RHO4)
RHOHAT = AK * AP
C4 = FOURPI /(AK * AK)
CSP = 0.0
C
C Compute potential scattering and phase factors
C
DO 1 LP = 1, 3
    AL = LP - 1
    IF(LP .EQ. 1) FI = RHOHAT
    IF(LP .EQ. 2) FI = RHOHAT - ATAN(RHOHAT)
    IF(LP .EQ. 3) FI = RHOHAT - ATAN(3.0 *
1   RHOHAT/(3.0 - RHOHAT * RHOHAT))
    CSP = CSP +(AL + AL + 1.0) * C4 * SIN(FI) * SIN(FI)
    TWOIFI = FI + FI
    SIN2FI(LP) = SIN(TWOIFI)
    COS2FI(LP) = COS(TWOIFI)
1 CONTINUE
DELTA = SQRT(AKB * TEMP * EREF / AW)
IF ( TEMP .EQ. 0.0 ) THEN
C
C Set coefficients for unbroadened cross sections
C
    DEN = 1.0
    CO = C4 / 4.0
ELSE
C
C Set coefficients for broadening cross sections
C
    DEN = DELTA
    TWODEL = DELTA + DELTA
    CO = ROOTPI * C4 / TWODEL
ENDIF
C
C Read unresolved resonance parameters and FILE 3 Contributions
C
    WRITE(1, 1002)
    CSD = 0.0
    JS = 0
C
    TYPE *, 'Type L, G, D, GO, GC, FW, NUM, NUF (D=0 => end data)'
C
2 CONTINUE
C
    ACCEPT 101, L, G, D, GO, GC, FW, NUM, NUF
C
    IF(D .EQ. 0.0) GO TO 3
    IF(NUM .EQ. 0) NUM = 1
C
    WRITE(1, 1003) L, G, D, GO, GC, FW, NUM, NUF
C
    Normalization factors ( Gaussian & Chi-squared distribution )
C
    GO = GO / NUM

```

```

IF(NUF .NE. 0) FW = FW / NUF
C
JS = JS + 1
LS(JS) = L + 1
GS(JS) = G
DS(JS) = CTP * D / DEN
GG(JS) = GC
GN(JS) = GO * V(L+1) * RTEREF
GF(JS) = FW
NN(JS) = NUN
NF(JS) = NUF
TGAM = GG(JS) + GN(JS) + GF(JS)
CSD = CSD + G * GN(JS) / TGAM
GO TO 2
3 CONTINUE
C
TYPE *, 'Enter with FILE 3 Contribution: CST3, CSC3, CSF3'
ACCEPT 102, CST3, CSC3, CSF3
C
WRITE(1, 1004) CST3, CSC3, CSF3
C
C
C Read probability-table limits or a blank card for default value.
C Default value calculated according to J. H. Otter et all.
C (AI-AEC-13024)
C
TYPE *, 'Type NPT, CSMIN, CSMAX or zero for default value'
ACCEPT 103, NPT, CSMIN, CSMAX
C
IF(NPT .LE. 0) NPT = 22
TMP = 0.2
IF(LS(2) .EQ. 1) TMP = 0.7
IF(CSMIN .LE. 0.0) CSMIN = TMP * CSP + CST3
IF(CSMAX .LE. 0.0) CSMAX = CSP + 6.0 * C4 * CSD + CST3
C
WRITE(1, 1005)
WRITE(1, 1006) NPT, CSMIN, CSMAX
C
ANP = NPT - 2
TERM = ANP / ALOG(CSMAX/CSMIN)
ALCSMN = ALOG(CSMIN)
C
C Initialize probability-table entries
C
DO 4 K = 1, NPT
    PT(K) = 0.0
    CSTK(K) = 0.0
    CSCK(K) = 0.0
    CSFK(K) = 0.0
4 CONTINUE
C
C Loop over number of cases
C
DO 12 N = 1, NL
    CST = 0.0
    CSC = 0.0
    CSF = 0.0
C
C Loop over J-L states
C
DO 8 J = 1, JS

```

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```

X = DS(J) * SQRT(RNMAXF(1.0))
XI(1) = -X * RAN(SEED)
XI(2) = X + XI(1)
LP = LS(J)
GC = GG(J)
NUN = NN(J)
NC2 = NUN + NF(J)

C
C      Two levels per pair
C
DO 7 IP = 1, 2
    SIGN = -SIGN
C
C      Loop over pairs
C
    DO 7 I = 1, IPAIRS
        IF(I .EQ. 1) XI = XI(IP)
        IF(I .GT. 1) XI = XI + SIGN * DS(J) *
*           SQRT(-ALOG(AMAX1(RAN(SEED), 0.00001)))
        G1 = 0.0
        FW = 0.0
        DO 6 NC = 1, NC2
            CONTINUE
            R1 = -ALOG(AMAX1(RAN(SEED), 0.00001))
            R2 = -ALOG(AMAX1(RAN(SEED), 0.00001))
            IF( R1 + R1 .LT. (R2-1.) * (R2-1.) ) GO TO 5
            IF(NC .LE. NUN) G1 = G1 + R2 * R2 * GN(J)
            IF(NC .GT. NUN) FW = FW + R2 * R2 * GF(J)
6       CONTINUE
        T1 = GC + G1 + FW
        IF ( TEMP .EQ. 0.0 ) THEN
C
C      Unbroadened cross sections
C
        TPT = XI * XI + T1 * T1 / 4.0
        CST = CST + G1 * ( T1 * COS2FI(LP) - 2.0 * XI *
*           SIN2FI(LP) ) * GS(J) / TPT
        CSC = CSC + G1 * GC * GS(J) / TPT
        CSF = CSF + G1 * FW * GS(J) / TPT
        ELSE
C
C      Broadened cross sections
C
        Y1 = T1 / TWODEL
        CALL SVS(X1, Y1, U1, V1)
        CST = CST + G1 * (U1 * COS2FI(LP) - V1 * SIN2FI(LP)) *
*           GS(J)
        CSC = CSC + GC * G1 * U1 * GS(J) / T1
        CSF = CSF + FW * G1 * U1 * GS(J) / T1
        END IF
7     CONTINUE
8     CONTINUE
        CST = CSP + CO * CST + CST3
        CSC = CO * CSC + CSC3
        CSF = CO * CSF + CSF3
        IF(CST .LE. CSMIN) GO TO 9
        IF(CST .GE. CSMAX) GO TO 10
        K = TERM * (ALOG(CST) - ALCSMN) + 2
        GO TO 11
9     CONTINUE
        K = 1

```

```

      GO TO 11
10   CONTINUE
      K = NPT
11   CONTINUE
      PT(K) = PT(K) + 1.0
      CSTK(K) = CSTK(K) + CST
      CSCK(K) = CSCK(K) + CSC
      CSFK(K) = CSFK(K) + CSF
12   CONTINUE
C
C   Construct probability-table, compute average cross-sections
C
      CSTB = 0.0
      CSCB = 0.0
      CSFB = 0.0
      CSTV = 0.0
      CSCV = 0.0
      CSFV = 0.0
      ANL = NL
C
      WRITE(1,1007)
C
      DO 13 K = 1, NPT
         IF(PT(K) .LE. 0.0 .OR. PT(K) .GE. ANL) GO TO 13
         PTK = PT(K)
         CST = CSTK(K)/PTK
         CSC = CSCK(K)/PTK
         CSF = CSFK(K)/PTK
         PTK = PTK/ANL
         PVK = PTK * (1.0 - PTK)/ANL
         PEK = SQRT(PVK)
         CSTB = CSTB + PTK * CST
         CSCB = CSCB + PTK * CSC
         CSFB = CSFB + PTK * CSF
         CSTV = CSTV + PTK * CST * CST
         CSCV = CSCV + PTK * CSC * CSC
         CSFV = CSFV + PTK * CSF * CSF
         CSTK(K) = CST
         CSCK(K) = CSC
         CSFK(K) = CSF
         PT(K) = PTK
C
         WRITE(1,1008) K, PTK, PEK, CST, CSC, CSF
C
13   CONTINUE
      CSTV = (CSTV - CSTB * CSTB)/ANL
      CSCV = (CSCV - CSCB * CSCB)/ANL
      CSFV = (CSFV - CSFB * CSFB)/ANL
      CSTE = SQRT(CSTV)
      CSCE = SQRT(CSCV)
      CSFE = SQRT(CSFV)
C
      WRITE(1,1009) CSTB, CSTE, CSCB, CSCE, CSFB, CSFE
C
C   Calculation of self-indication and transmission ratios
C
      TYPE *, 'Type thicknesses. Up to ten values or a blank card if it i
      *s not needed.'
      ACCEPT 104, (SIGDIL(M), M = 1, 10)

```

18 Appendix A. FORTRAN LISTING OF URR

```

C      IF(SIGDIL(1) .EQ. 0.0) GO TO 17
C      WRITE(1,1011)
C
C      Loop over transmissions
C
C      DO 16 M = 1, 10
      SIGO = SIGDIL(M)
      IF(SIGO .EQ. 0.0) GO TO 16
      ANUM = 0.0
      ADEN = 0.0
      TRMO = 0.0
      TRM1 = 0.0
      TRM2 = 0.0
      FNUM = 0.0
      FDEN = 0.0
      FRMO = 0.0
      FRM1 = 0.0
      FRM2 = 0.0
      TRAN = 0.0
      TRN2 = 0.0
C
C      Loop over probability-table entries
C
C      DO 14 K = 1, NPT
      PTK = PT(K)
      IF(PTK .EQ. 0.0) GO TO 14
      CST = CSTK(K)
      CSC = CSCK(K)
      CSF = CSFK(K)
      EXPT = EXP(-SIGO * CST)
      TERM = PTK * CSC
      FERM = PTK * CSF
      ANUM = ANUM + TERM * EXPT
      FNUM = FNUM + FERM * EXPT
      ADEN = ADEN + TERM
      FDEN = FDEN + FERM
      TRMT = PTK * EXPT
      TRAN = TRAN + TRMT
      TSQR = TERM * CSC
      FSQR = FERM * CSF
      TRMO = TRMO + TSQR
      FRMO = FRMO + FSQR
      TRM1 = TRM1 + TSQR * EXPT
      FRM1 = FRM1 + FSQR * EXPT
      TRM2 = TRM2 + TSQR * EXPT * EXPT
      FRM2 = FRM2 + FSQR * EXPT * EXPT
      TRN2 = TRN2 + TRMT * EXPT
14    CONTINUE
      ETR = SQRT((TRN2 - TRAN * TRAN)/ANL)
      SSCSC = ANUM/ADEN
      VAR = (TRM2 + SSCSC * SSCSC * TRMO -
* (SSCSC + SSCSC) * TRM1)/(ADEN * ADEN * ANL)
      ER = SQRT(VAR)
      IF(FDEN .EQ. 0.0) GO TO 15
      SSFSC = FNUM/FDEN

```

```

      VFR = (FRM2 + SSFSC * SSFSC * FRM0 -
* (SSFSC + SSFSC) * FRM1)/(FDEN * FDEN * ANL)
      FR = SQRT(VFR)
15    CONTINUE
C
      WRITE(1,1012) SIG0, SSCSC, ER, SSFSC, FR, TRAN, ETR
C
16    CONTINUE
C
17    CONTINUE
C
C Calculation of Bondarenko partial and transport cross sections
C
      TYPE *, 'Type sigma dilutions. Up to ten values or a blank card if
* it is not needed.'
      ACCEPT 104, (SIGDIL(M), M = 1, 10)
C
      IF(SIGDIL(1).EQ.0.) GO TO 20
C
      WRITE(1, 1013)
C
C Loop over dilutions
C
      DO 19 M = 1, 10
      SIG0 = SIGDIL(M)
      IF(SIG0 .EQ. 0.0) GO TO 19
      ANUM = 0.0
      FNUM = 0.0
      ADEN = 0.0
      TRMO = 0.0
      TRM1 = 0.0
      TRF1 = 0.0
      TRM2 = 0.0
      TRF2 = 0.0
      ANUT = 0.0
      ADET = 0.0
      CST1 = 0.0
      CST2 = 0.0
C
C Loop over probability-table entries
C
      DO 18 K = 1, NPT
      PTK = PT(K)
      IF(PTK .EQ. 0.0) GO TO 18
      CST = CSTK(K)
      CSC = CSCK(K)
      CSF = CSFK(K)
      TERM = PTK/(CST + SIG0)
      ANUM = ANUM + TERM * CSC
      FNUM = FNUM + TERM * CSF
      ADEN = ADEN + TERM
      TSQR = TERM/(CST + SIG0)
      ANUT = ANUT + TERM
      ADET = ADET + TSQR
      TRMO = TRMO + TSQR
      TRM1 = TRM1 + TSQR * CSC
      TRF1 = TRF1 + TSQR * CSF
      TRM2 = TRM2 + TSQR * CSC * CSC
      TRF2 = TRF2 + TSQR * CSF * CSF
      CST1 = CST1 + CST * PTK
      CST2 = CST2 + CST * CST * PTK

```

20 Appendix A. FORTRAN LISTING OF URR

```

18      CONTINUE
      SSCSC = ANUM/ADEN
      SSFSC = FNUM/ADEN
      VAR = (TRM2 + SSCSC * SSCSC * TRMO -
* (SSCSC + SSCSC) * TRM1)/(ADEN * ADEN * ANL)
      VFR = (TRF2 + SSFSC * SSFSC * TRMO -
* (SSFSC + SSFSC) * TRF1)/(ADEN * ADEN * ANL)
      ER = SQRT(VAR)
      FR = SQRT(VFR)
      TRAN = ANUT/ADET - SIGO
      ETR = SQRT((CST2 + TRAN * TRAN -2.0 * TRAN * CST1)/ANL)
C
      WRITE(1,1014) SIGO, SSCSC, ER, SSFSC, FR, TRAN, ETR
C
19      CONTINUE
20      CONTINUE
      STOP
C
C      Input format list
C
100   FORMAT(6F, 3I)
101   FORMAT(I, 6F, 2I)
102   FORMAT( 3F )
103   FORMAT(I, 3F)
104   FORMAT(10F)
C
C      Output format list
C
1000  FORMAT('0          AW          AWRI          AP
* ENER        TEMP        NCASES        NPAIRS')
1001  FORMAT(1H , 5G16.5, 5I8///)
1002  FORMAT('0                               J-STATES'
*'     L          G          D          GO
*'     GC         FW         NUN NUF')
1003  FORMAT(18 , 5G17.5, 2I4)
1004  FORMAT(///'          TOTAL          CAPTURE          FILE 3 CONTRIBU
*'          / 3G20.5///'          / 3G20.5///'          FISSION
1005  FORMAT('0 NUMBER OF PT ENTRIES          CSMIN          CSMAX')
1006  FORMAT(6X, 18 , 5X, 5G20.5///)
1007  FORMAT('0          K          PK          PROBABILITY-TABLE'
*'          CSC          CSF          CST
1008  FORMAT(18 , 5G20.5)
1009  FORMAT(///'          AVERAGE TOTAL CROSS SECTION  ',G16.5,'+/-',G16.5/
*'          AVERAGE CAPTURE CROSS SECTION ',G16.5. ' +/-',G16.5/
*'          AVERAGE FISSION CROSS SECTION ',G16.5,'+/-',G16.5)
1010  FORMAT(1H ,7G16.5)
1011  FORMAT(///'          SELF INDICATION AND TRANSMISSIO
*'          RATIO')
1012  FORMAT(///'          THICKNESS ',G16.5/' C
*'          CAPTURE SELF INDICATION RATIO ',G16.5.'+/-',G16.5/' FISSION SELF IN
*'          DICATION RATIO ',G16.5.'+/-',G16.5/'          TRANSMISSION
*'          ',G16.5.'+/-',G16.5)
1013  FORMAT(///'          SELF SHIELDING CROSS SECTIONS')
1014  FORMAT(///'          DILUTION ',G16.5/' C
*'          CAPTURE CROSS SECTION  ',G16.5.'+/-',G16.5/' FISSION CROSS SECTION
*'          ',G16.5.'+/-',G16.5/' TRANSPORT CROSS SECTION ',G16.5.'+/-'
*,G16.5)
      END
      SUBROUTINE SVS(A, B, C, D)

```

```

COMMON/TRTI/ TR(62,62), TI(62,62), AIMW, AX, KI, REW, Y1
DOUBLE PRECISION A, B, C, D
DATA K/0/
IF(K .EQ. 1) GO TO 3
K = 1
KI = 1
X = -0.1
DO 2 I = 1, 62
    Y = -0.1
    DO 1 J = 1, 62
        CALL W(X, Y, TR(I,J), TI(I,J))
        Y = Y + 0.1
    1    CONTINUE
    X = X + 0.1
2    CONTINUE
3    CONTINUE
AX = A
Y1 = B
CALL QUICKW
C = REW
D = AIMW
RETURN
END
SUBROUTINE W(REZ,AIM1,REW,AIMW)
C
C Subroutine W and QUICKW are taken from H. Henryson II et all (MC-2).
C (ANL-8144)
C
REW = 0.0
AIMW = 0.0
AIMZ = ABS(AIM1)
IF(REZ) 3, 1, 3
1 IF(AIM1) 3, 2, 3
2 REW = 1.0
RETURN
3 R2 = REZ * REZ
AI2 = AIMZ * AIMZ
ABREZ = ABS(REZ)
IF(ABREZ + 1.25 * AIMZ - 5.0) 6, 6, 4
4 IF(ABREZ + 1.1 * AIMZ - 6.6) 21, 21, 20
5 IF(ABREZ + 1.43333 * AIMZ - 4.3) 23, 23, 22
6 IF(ABREZ + 1.863636 * AIMZ - 4.1) 15, 15, 8
7 IF(AIMZ - 1.6) 14, 24, 24
8 IF(AIMZ - 1.4) 19, 19, 5
9 IF(ABREZ + 1.07317 * AIMZ - 4.4) 23, 23, 22
10 IF(ABREZ - 2.7) 31, 32, 32
11 IF(ABREZ - 3.1) 10, 12, 12
12 IF(ABREZ - 3.4) 33, 34, 34
13 IF(R2 + 1.18 * AI2 - 5.76) 7, 11, 11
14 IF(R2 + 1.7227 * AI2 - 4.41) 29, 30, 30
15 IF(R2 + 1.71 * AI2 - 2.89) 17, 13, 13
16 IF(R2 + 1.69 * AI2 - 1.69) 27, 28, 28
17 IF(R2 + 2.0408 * AI2 - 1.0) 18, 16, 16
18 IF(R2 + 1.5625 * AI2 - 0.25) 25, 26, 26
19 IF(ABREZ + 1.43333 * AIMZ - 4.3) 24, 24, 9
20 NMAX = 1
GO TO 36
21 NMAX = 2
GO TO 36
22 NMAX = 3
GO TO 36

```

22 Appendix A. FORTRAN LISTING OF URR

```

23   NMAX = 4
24   GO TO 36
25   NMAX = 6
26   GO TO 36
27   NMAX = 2
28   GO TO 35
29   NMAX = 3
30   GO TO 35
31   NMAX = 4
32   GO TO 35
33   NMAX = 5
34   GO TO 35
35   NMAX = 6
36   GO TO 35
37   NMAX = 7
38   GO TO 35
39   NMAX = 8
40   GO TO 35
41   NMAX = 9
42   GO TO 35
43   NMAX = 10
44   GO TO 35
45   NMAX = 11
46   KW = 2
47   AIMZ = AIM1
48   GO TO 44
49   KW = 1
50   IF(AIM1) 37, 38, 39
51   KW = 2
52   AIMZ = AIM1
53   GO TO 44
C
C
C WA IS OBTAINED FROM ASYMPTOTIC SERIES
C
C
38   RV = 2.0 * (R2 - AI2)
      AK = 4.0 * REZ * AIMZ
      EL = AK
      H = 0.0
      B = 0.0
      A = 0.0
      TEMPM = 0.0
      TEMEL = 0.0
      G = 1.0
      C = -1.1283792 * AIMZ
      D = 1.1283792 * REZ
      AM = RV - 1.0
      AAK = 1.0
      K = 0
39   AJTEMP = 2.0 * AAK
      TEMP4 =(1.0 - AJTEMP) * AJTEMP
      AJP = RV - (4.0 * AAK + 1.0)
      GO TO 51
40   AAK = AAK + 1.0
      K = K + 1
      PR = REW
      PI = AIMW
41   AMAGN = TEMP4*TEMPM + TEMEL*TEMEL
      REW = (TEMP4 * TEMP4 + TEMPD * TEMEL)/AMAGN
      AIMW = (TEMPM * TEMPD - TEMEL * TEMP4)/AMAGN

```

```

        IF(ABS(REW - PR) - 1.E-6) 42, 39, 39
42    IF(ABS (AIMW - PI) - 1.E-6) 43, 39, 39
43    RETURN
C
C
C WT IS OBTAINED FROM TAYLOR SERIES
C
C
44    TEMP1 = R2 + AI2
        TEMP2 = 2.0 * TEMP1 * TEMP1
        AJ = -(R2 - AI2)/TEMP2
        AK = 2.0 * REZ * AIMZ/TEMP2
        C = 0.0
        B = 0.0
        AJSIG = 0.0
        D = 0.0
        JSIG = 0
        G = 0.0
        H = 0.0
        EL = 0.0
        A = 1.0
        AM = 1.0
        SIGP = 1.5
        EXPON = EXP(TEMP2 * AJ)
        EXPC = EXPON * COS(TEMP2 * AK)
        EXPS = -EXPON * SIN(TEMP2 * AK)
        SIG2P = 2.0 * SIGP
45    AJ4SIG = 4.0 * AJSIG
        AJ4SM1 = AJ4SIG - 1.0
        TEMP3 = 1.0/(AJ4SM1 * (AJ4SIG + 3.0))
        TT4 = SIG2P * (2.0 * AJSIG - 1.0)
        TEMP4 = TT4/(AJ4SM1 * (AJ4SIG + 1.0) * (AJ4SIG - 3.0) * AJ4SM1)
        AJP = AJ + TEMP3
        GO TO 51
46    AJSIG = AJSIG + 1.0
        JSIG = JSIG + 1
47    TEMP7 = (AM * AM + EL * EL) * 1.7724539
        REF = (AIMZ * (C * AM + D * EL) - REZ * (AM * D - C * EL))/*
        * TEMP7/TEMP1
        AIMF = (AIMZ * (AM * D - C * EL)) + REZ *
        * (C * AM + D * EL))/TEMP7/TEMP1
        PR = REW
        PI = AIMW
        REW = EXPC - REF
        AIMW = EXPS - AIMF
        IF(ABS(REW - PR) - 1.E-6) 48, 50, 50
48    IF(ABS (AIMW - PI) - 1.E-6) 49, 50, 50
49    RETURN
50    SIG2P = 2.0 * AJSIG
        GO TO 45
51    TEMPC = AJP * C + TEMP4 * A - AK * D
        TEMPD = AJP * D + TEMP4 * B + AK * C
        TEMEL = AJP * EL + TEMP4 * H + AK * AM
        TEMPN = AJP * AM + TEMP4 * G - AK * EL
        A = C
        B = D
        G = AM
        H = EL
        C = TEMPC
        D = TEMPD
        AM = TEMPN

```

```

EL = TEMEL
IF(ABS(TEMPM) + ABS(TEMEL) - 1.0E15) 53, 52, 52
52  C = 1.0E-15 * C
D = 1.0E-1 * D
AM = 1.0E-15 * AM
EL = 1.0E-15 * EL
TEMPC = 1.0E-15 * TEMPc
TEMPD = 1.0E-15 * TEMPD
TEMPM = 1.0E-15 * TEMPM
TEMEL = 1.0E-15 * TEMEL
GO TO 55
53  IF(ABS(TEMPM) + ABS(TEMEL) - 1.0E-15) 54, 54, 55
54  C = 1.0E15 * C
D = 1.0E15 * D
AM = 1.0E15 * AM
EL = 1.0E15 * EL
TEMPC = 1.0E15 * TEMPc
TEMPD = 1.0E15 * TEMPD
TEMPM = 1.0E15 * TEMPM
TEMEL = 1.0E15 * TEMEL
55  GO TO(40, 46, 56), KW
56  RETURN
END
SUBROUTINE QUICKW
COMMON/TRTI/ TR(62, 62), TI(62,62), AIMW, AX, KI, REW, Y
AKI = SIGN(1.0, AX)
X = ABS(AX)
TEST = X * X + Y * Y
IF(TEST .LT. 36.0) GO TO 1
IF(TEST .LT. 144.0) GO TO 4
IF(TEST .LT. 10000.0) GO TO 6
A1 = 1.0/(1.7724539 * TEST)
REW = Y * A1
IF(KI .GT. 0) AIMW = X * A1 * AKI
RETURN
1   II = X * 10.0
JJ = Y * 10.0
I = II + 2
J = JJ + 2
N = J - 1
P = 10.0 * X - II
Q = 10.0 * Y - JJ
2   P2 = P * P
Q2 = Q * Q
PQ = P * Q
HP = 0.5 * P
HQ = 0.5 * Q
HQ2 = 0.5 * Q2
HP2 = 0.5 * P2
A1 = HQ2 - HQ
A2 = HP2 - HP
A3 = 1.0 + PQ - P2 - Q2
A4 = HP2 - PQ + HP
A5 = HQ2 - PQ + HQ
REW = A1 * TR(I,N) + A2 * TR(I-1,J) + A3 * TR(I,J) + A4 *
* TR(I+1,J) + A5 * TR(I,J+1) + PQ * TR(I+1,J+1)
IF(KI.LE.0) GO TO 8
3   AIMW = A1 * TI(I,N) + A2 * TI(I-1,J) + A3 * TI(I,J) + A4 *
* TI(I+1,J) + A5 * TI(I,J+1) + PQ * TI(I+1,J+1)
AIMW = AIMW * AKI
GO TO 8

```

```

4   A1 = X * X - Y * Y
A2 = 2.0 * X * Y
A3 = A2 * A2
A4 = A1 - 0.2752551
A5 = A1 - 2.724745
D1 = 0.5124242/(A4 * A4 + A3)
D2 = 0.05176536/(A5 * A5 + A3)
REW = D1 *(A2 * X - A4 * Y) + D2 *(A2 * X - A5 * Y)
IF(KI .LE. 0) GO TO 8
5   AIMW = D1 * (A4 * X + A2 * Y) + D2 * (A5 * X + A2 * Y)
AIMW = AIMW * AKI
GO TO 8
6   A1 = (X * X - Y * Y) * 2.0
A2 = 4.0 * X * Y
A4 = A1 - 1.0
D1 = 1.1283792/(A4 * A4 + A2 * A2)
REW = D1 * (A2 * X - A4 * Y)
IF(KI .LE. 0) GO TO 8
7   AIMW = D1 * (A4 * X + A2 * Y)
AIMW = AIMW * AKI
8   RETURN
END
FUNCTION RNMAXF(T)
DATA FF/0.0/
INTEGER*4 SEED
COMMON SEED
U= EXPRNF(U)
IF(FF) 3, 1, 3
1   R1 = RAN(SEED)
R2 = RAN(SEED)
R1SQ = R1 * R1
R2SQ = R2 * R2
RSQ = R1SQ + R2SQ
IF(RSQ - 1.0) 2, 2, 1
2   W = EXPRNF(W)/RSQ
FF = 1.0
RNMAXF = (R2SQ * W + U) * T
GO TO 4
3   FF = 0.0
RNMAXF = (R1SQ * W + U) * T
4   RETURN
END
FUNCTION EXPRNF(A)
REAL I
INTEGER*4 SEED
COMMON SEED
I = 0.0
1   X = RAN(SEED)
Z = X
2   Y = RAN(SEED)
IF(Z - Y) 5, 5, 3
3   Z = RAN(SEED)
IF(Z - Y) 2, 4, 4
4   I = I + 1.0
GO TO 1
5   EXPRNF = X + I
RETURN
END

```

APPENDIX B. SAMPLE CASE

a. Listing of Input

```

$RUN URR
Output file name. (Default is OUTPUT.URR)
OUT.DAT
TYPE AW, AWRI, AP, EREF, TEMP, NL, IPAIRS, SEED
235.0,233.0351,0.93811,150.0,300.0,10000,2,19
Type L, G, D, GO, GC, FW, NUM, NUF (D=0 => end data)
0,0.4375,1.39,0.1217E-3,38.0E-03,268.0E-03,1,2
0,0.5625,0.90,0.0914E-3,35.0E-03,226.0E-03,1,2
Enter with FILE 3 Contribution: CST3, CSC3, CSF3
Type NPT, CSNIN, CSMAX or zero for default value
Type thicknesses. Up to ten values or a blank card if it is not needed.
0.0325,0.0
Type sigma dilutions. Up to ten values or a blank card if it is not needed.
100.0,0.0

```

b. Listing of output

NCASES	AW		AWRI		AP		ENER		TEMP	
	NPairs									
10000	235.00		233.04		0.93811		150.00		300.00	
	J-STATES									
	L	G		D		GO		GC		
FW	NUN	NUF								
0.26800	0	0.43750		1.3900		0.12170E-03		0.38000E-01		
0.22600	0	0.56250		0.90000		0.91400E-04		0.35000E-01		
	1	2								
	FILE 3 CONTRIBUTIONS									
	TOTAL		CAPTURE		FISSION					
	0.00000E+00		0.00000E+00		0.00000E+00					
NUMBER OF PT ENTRIES			CSMIN		CSMAX					
22			7.7397		849.54					
	PROBABILITY-TABLE									
	K	PK		ERROR		CST		CSC		
CSF										
0.86194	3	0.15800E-01		0.12470E-02		11.921		0.28793		
2.4752	4	0.10930		0.31202E-02		14.086		0.68068		
5.2628	5	0.14050		0.34751E-02		17.662		1.3744		
8.7743	6	0.14240		0.34946E-02		22.310		2.3521		
13.287	7	0.12640		0.33230E-02		28.153		3.6473		
18.913	8	0.12030		0.32531E-02		35.665		5.3825		
25.665	9	0.10310		0.30409E-02		45.003		7.7592		
34.431	10	0.76100E-01		0.26516E-02		56.891		10.649		

Appendix B. SAMPLE CASE 27

11	0.61300E-01	0.23988E-02	71.855	15.199
44.416				
12	0.44600E-01	0.20642E-02	90.872	20.384
57.213				
13	0.31100E-01	0.17359E-02	114.32	27.740
72.302				
14	0.15900E-01	0.12509E-02	144.54	38.276
89.301				
15	0.79000E-02	0.88530E-03	183.20	49.273
113.04				
16	0.35000E-02	0.59057E-03	227.99	71.485
128.53				
17	0.13000E-02	0.36032E-03	283.10	85.399
161.09				
18	0.30000E-03	0.17318E-03	398.92	118.17
225.50				
19	0.20000E-03	0.14141E-03	450.62	189.57
188.60				
AVERAGE TOTAL CROSS SECTION	41.339	+/-	0.34656	
AVERAGE CAPTURE CROSS SECTION	7.4618	+/-	0.10162	
AVERAGE FISSION CROSS SECTION	22.095	+/-	0.22847	
SELF INDICATION AND TRANSMISSION RATIOS				
THICKNESS	0.32500E-01			
CAPTURE SELF INDICATION RATIO	0.15909	+/-	0.23306E-02	
FISSION SELF INDICATION RATIO	0.18470	+/-	0.21449E-02	
TRANSMISSION	0.36139	+/-	0.19660E-02	
SELF SHIELDING CROSS SECTIONS				
DILUTION	100.00			
CAPTURE CROSS SECTION	5.8873	+/-	0.63333E-01	
FISSION CROSS SECTION	18.263	+/-	0.16308	
TRANSPORT CROSS SECTION	31.754	+/-	0.35958	

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