International Atomic Energy Agency

INDC(CSR)-016/LJ

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PEQAG: A PC VERSION OF FULLY PRE-EQUILIBRIUM COMPUTER CODE WITH GAMMA EMISSION*

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* The work has been performed under IAEA CRP on "Development of Improved Formalism in the Frame of Pre-equilibrium/compound Nuclear Reaction Theory and Code for Particle and Gamma Emission Spectra at Medium Excitation Energies" and research contract No. 5148/RB.

June 1989

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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June 1989

89-02378

I. CHARACTERISTICS OF THE PROGRAM

Purpose of the program: Exciton model calculation of angle-integrated nucleon and γ energy spectra. All the emissions are treated consistently within the pre-equilibrium approach based on the master equations of the model. Multiple particle and/or multiple γ emissions are included.

Quantities calculated : Angle-integrated energy spectra of neutrons, protons, and γ, as well as the corresponding integrals. No angle-dependent or spin-dependent calculations are included.

Channels considered : n, p, γ, and their combinations.

State density used : Equidistant-spacing model in the finite potential well with g=A/13 for all nuclei.

Inverse cross sections: Supplied by the program according to the approximation of Chatterjee et al. The GDR shape is described as a Lorentzian one with global parameters. The replacement of the program built-in options by some other form of cross sections (or an input of them) is trivial.

Neutron/proton distinguishability: One-component description with R-factor of Cline for an approximate accounting of the two-component nature.

Number of successive emissions: Up to 4 nucleons emitted and interspersed and/or preceded by arbitrary number of gammas. (This value can be easily changed by simple adjusting of the dimensions of arrays.)

Maximum energy possible:	68 times the energy step used. (This can be easily changed by proper redimensioning the arrays.)	
Size of the program :	Source	649 lines (21 kB)
	Object code	22 kB
	Exe form	271 kB
Time	Compilation	2´
	Test run calculation	3´ 10´´
	(Time refers to PC/AT and MS Fortran version 3.31.)	
Warning	The use of double precision within the program is necessary.	
Relation to other programs:	This program is somewhat updated version of the PEQGM code [1], transferred to IBM PC computers.	

II. Basic equations

The pre-equilibrium decay is (within its exciton model) governed by the set of master equations. In order to be able to handle properly also cascades of γ quanta in the model, the set of master equations (usually several tens of coupled equations) of the exciton model was enlarged as to couple different excitation energies and even various nuclei [1, 2]. This means we are able to describe the γ emission within the same formalism up to the total de-excitation of a nucleus, independently of a possible particle emission prior to or between the successive γ´s. The corresponding enlarged set of master equations reads

$$\begin{aligned}\frac{dP(n,t,E,i)}{dt} &= P(n-2,t,E,i)\,\lambda^{+}(n-2,E,i) \\ &+ P(n+2,t,E,i)\,\lambda^{-}(n+2,E,i) \\ &- P(n,t,E,i)\,[\lambda^{+}(n,E,i) + \lambda^{-}(n,E,i) + L(n,E,i)] \\ &+ \sum_{j,m,\kappa} \int_{\varepsilon} P(m,t,E',j)\,\lambda^{c}_{\kappa}(m,E',j,\varepsilon)\,d\varepsilon\,. \qquad (1)\end{aligned}$$

In eqs. (2), $P(n,t,E,i)$ is the occupational probability of an n-exciton state of a nucleus i at the excitation energy E

and time t, λ's are the transition rates (per unit time) to the neighbour states, and L is the total emission rate (including particles and gammas, integrated over the outgoing energy and summed over all possible emission channels) of the specified exciton state,

$$L(n,E,i) = \sum_{x} \int_{\varepsilon} P(n,t,E,i)\, \lambda_{x}^{c}(n,E,i,\varepsilon)\, d\varepsilon \ . \qquad (2)$$

The last term in eq. (2) ensures the coupling of different nuclei and various excitation energies. The transition as well as the emission rates depend on the densities of n-exciton states in a given nucleus (the composite and the residual one). These densities are usually approximated within the equidistant-spacing scheme, what leads to the Ericson-type formulas. Explicit treatment of the Pauli principle (two excitons cannot share the same level) results in nonanalytical expressions, which can be well reproduced by the Williams formula [3]

$$\omega(p,h,E) = \frac{g \cdot (gE-A_{ph})^{p+h-1}}{p!\ h!\ (p+h-1)!} \qquad (3)$$

where we have put separately the particle (p) and the hole (h) numbers (totally giving the exciton number, $n = p + h$). A_{ph} stands for the correction term due to the Pauli principle,

$$A_{ph} = \frac{p^2 + p + h^2 - 3h}{4\ g} \ . \qquad (4)$$

For higher energies, the densities are modified as to take into account the finite depth of the nuclear potential well [4]. The transition rates are [5, 6]

$$\lambda^{+}(n,E) \approx \frac{2\pi}{\hbar} |M|^2 \frac{g \cdot (gE-A_{ph})^2}{2\ (n+1)}$$

$$\lambda^{-}(n,E) \approx \frac{2\pi}{\hbar} |M|^2 \frac{g}{2} \cdot ph(n-2). \qquad (5)$$

Here, the appearance of an extra factor of 2 in the denominator is due to the indistinguishability of particles (holes). The nucleon emission rates are in their standard form [7]

$$\lambda^{c}_{x}(n,E,\varepsilon_{x})\,d\varepsilon_{x} = \frac{2s_{x}+1}{\pi^{2}\hbar^{3}}\,\mu_{x}\,\varepsilon_{x}\,\sigma^{*}_{INV}(\varepsilon_{x})\,\frac{\omega_{R}(n-1,U)}{\omega(n,E)}\,R_{x}(n)\,d\varepsilon_{x}. \quad (6)$$

The symbols in (6) have their usual meaning, $R_{x}(n)$ is the effective factor, which simulates the two-component nature of the problem (for every n-exciton state $R_{p}+R_{n}=1$). The γ emission rate λ^{c}_{γ} is given [8, 9]

$$\lambda^{c}_{\gamma}(n,E,\varepsilon_{\gamma}) = \frac{\varepsilon_{\gamma}^{2}\sigma_{a}(\varepsilon_{\gamma})}{\pi^{2}\hbar^{3}c^{2}}\,\frac{\sum_{m=n,n-2} b(m,\varepsilon_{\gamma})\,\omega(m,E-\varepsilon_{\gamma})}{\omega(n,E)} \quad (7)$$

with [9]

$$b(n-2,\varepsilon_{\gamma}) = \frac{\omega(1,1,\varepsilon_{\gamma})}{g(n-2)+\omega(1,1,\varepsilon_{\gamma})}$$

$$b(n,\varepsilon_{\gamma}) = \frac{g_{n}}{g_{n}+\omega(1,1,\varepsilon_{\gamma})}\,. \quad (8)$$

In eq. (7), $\sigma_{a}(\varepsilon_{\gamma})$ is the photoabsorption cross section, which can be taken e.g. in the form of the Lorentzian description of the giant dipole resonance. As all the interested physical quantities, like cross sections, spectra, etc. do not depend directly on $P(n,E,t)$'s, but only on their time integrals,

$$\tau(n,E) = \int_{0}^{\infty} P(n,E,t)\,dt\,, \quad (9)$$

we can formally integrate the eqs. (2) in time, replacing thus the set of differential equations by a set of the algebraic ones. The new set of equations with all necessary couplings for the γ emission reads [3, 6]

$$\begin{aligned} -D_{n,E,i} &= \tau(n-2\;E,i)\,\lambda^{+}(n-2,E,i) \\ &+ \tau(n+2,E,i)\,\lambda^{-}(n+2,E,i) \\ &- \tau(n,E,i)\,[\lambda^{+}(n,E,i)+\lambda^{-}(n,E,i)+L(n,E,i)] \\ &+ \sum_{j,m,x}\int_{\varepsilon} \tau(m,E',j)\,\lambda^{c}_{x}(m,E',j,\varepsilon)\,d\varepsilon. \end{aligned} \quad (2')$$

Here, $D_{n,E,i}$ is the initial exciton configuration of the composite system (taken to be $A_p p0h$, where A_p is the mass number of the projectile, and *1p1h* for the reactions induced by gammas). The transition matrix element $|M|^2$ is taken in its exciton number dependent form [10]. The standard value of the constant K for the transition matrix element is K=65 MeV^3 [10].

II. Input

First, the computer asks for the names of the input and the output data files. The input file consists of a set of 5 lines for one calculation:

1. *FMT 1X,79H* Title card of the calculation.
2. *FMT 3I4* IN, IZ, KEYO
   The neutron and the proton numbers of the composite nucleus, followed by the key number of the projectile (*1*-n, *2*-p, *3*-d, *4*-t, *5*-^{3}He, *6*-α, *7*-γ).
3. *FMT 4F8.* EEXCO, ESTEP, SGR, AK
   The excitation energy (MeV) of the composite system, the energy step (MeV) for the calculation, the reaction cross section (mb), and the constant for the matrix element (MeV^3). If SGR<0, the program approximates the cross section by the formula of Chatterjee et al. [11].
4. *FMT 10F4.* B
   Binding energies for neutrons in accord with the key numbers of the nuclei in the chain.
5. *FMT 10F4.* B *(continued)*
   Binding energies for protons in the same same order as above.

Arbitrary number of five-card sets can be combined in one program run. The calculation stops for IN+IZ=0.

Key numbers of the nuclei in the reaction chain: 0-originally created composite nucleus (A,Z), 1-(A-1,Z),

2-(A-1,Z-1), 3-(A-2,Z), 4-(A-2,Z-1), 5-(A-2,Z-2), 6-(A-3,Z), 7-(A-3,Z-1), 8-(A-3,Z-2), 9-(A-3,Z-3).

IV. OUTPUT

The program informs the user, which nucleus in the reaction chain is just being calculated, by corresponding information on the screen. The proper output is placed into the specified file.

The output starts with a head, which repeats nearly all the input information, and supplies some values calculated by the program itself (e.g. the GDR energy). Then the series of outputs for different nuclei (in the order specified above) appears. For each nucleus, two tables are edited:

The first table brings information on the master equation solution for a given nucleus, ordered (within this nucleus) in a decreasing value of the excitation energy. There are three integers (0,20, and 47) in the first line of the sample run, denoting the key of the nucleus (0), number of iterations performed (usually 20 near the beginning of the reactions, and 2 thereafter), and the excitation energy in the units of the energy step (47). The three floating point numbers, which follow, are the fraction of the particle emission, that of the gammas, and the total one (usually, the algorithm used deviates slightly from 1.0, but a manifestation of this error in the resulting spectra is minimized to less than 1 per cent). The next line brings the solutions of the master equation for given nucleus at specified excitation energy. This information is repeated for all energies of given nucleus; however, in the sample run copy the medium lines are missing.

The second table is the proper result of the calculation: the particle and γ energy (c.m.) spectra (in mb/MeV), followed by the corresponding integral cross sections. Note that for subsequent nuclei, only the emission from given nucleus is presented in this table, and <u>not</u> the summation from the beginning up to the given nucleus.

If the energy does not permit creation of a particular nucleus within the reaction chain, both the tables for such a nucleus are skipped.

V. Program listing and the sample run

The Appendices bring the complete program listing (Appendix A), the input file (Appendix B), and a part of the test run output (Appendix C) produced using the input from Appendix B.

The author is grateful to A. Perdan for his assistance at transfer the code from a mainframe computer to the PC.

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```
C       PROGRAM PEQAG (Akk.+Gr. basic version, 10 Jan 1989)
C
C       PROGRAM FOR PRE-EQUILIBRIUM CALCULATIONS WITHIN THE MASTER
C       EQUATION APPROACH.
C       ONLY NEUTRON, PROTON AND GAMMA EMISSION IS CALCULATED
C       MULTIPLE PARTICLE AND (VIRTUALLY) INFINITE-MULTIPLE GAMMA EMISSION
C       ARE INCORPORATED.
C       ALGORITHM PUBLISHED IN:  DOBES,BETAK: Z. PHYS. A288 (1978), 175
C       GAMMA EMISSION AS IN:  Akkermans, Gruppelaar: PL 157B (1985)
C
        IMPLICIT REAL*8 (A-H,O-Z)
        character*50 if,of,tit*70
        COMMON FAL(59),EF,IAC,IZC
        COMMON /MC/ IAO,IZO,KEY
        COMMON /GAM/ TO(25,68), OM(25,68), SG(3,68), AF,C2,ESTEP,G,T1111,
       1             IO, IAT, IEEXC, IEO, IZ, N
        DIMENSION T1(25, 68), T2( 5, 25, 68), ALP(25, 68), ALM(25, 68),
       1          TAU(25, 68), OMR(25, 68), SE(3, 68), R(2, 25, 10),
       2          EMP(25,68), EMG(25,68), B(10,2), IB(10,2), IXC(9)
@large
C
C       WRITTEN FOR ARBITRARY PROJECTILE. THE INVERSE CROSS SECTIONS
C       APPROXIMATED ACCORDING TO CHATTERJEE AND GUPTA
C
C       THE INITIAL EXCITON CONFIGURATION IS ASSUMED TO BE
C                                   HO=0, PO=A(PROJ)
C
C       KEYS:    0-GAMMA,   1-N,   2-P,   3-D,   4-T,   5-HE-3,   6-ALPHA
C
C       THE CHAIN OF THE NUCLEI WITHIN THE REACTION IS DENOTED VIA IIIIIO
C
C                                       0
C                                    CN(A,Z)
C
C                            1                    2
C                         (A-1,Z)              (A-1,Z-1)
C
C                 3                    4                    5
C              (A-2,Z)              (A-2,Z-1)            (A-2,Z-2)
C
C        6                    7                    8                    9
C     (A-3,Z)              (A-3,Z-1)            (A-3,Z-2)            (A-3,Z-3)
C
C       ARTERISKS DENOTE THE COMMANDS DEPENDING ON THE CHOICE OF (PO,HO)
C       * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
        write(*,1)
      1 format(' Input data file  ?    ',@)
        read(*,2) if
      2 format(a50)
      7 write(*,3)
      3 format(' Output list file ?    ',@)
        read(*,2) of
        open(5,file=if,status='old')
        open(6,file=of,status='new',err=7)
        PI=3.141593
        EF = 40.
        IR = 5
        IW = 6
        AK=65.
```

```
      FAL(1) = 0.
      FAL(2) = 0.
      FAL(3) = 0.
    6 format(1x,a30)
      DO 500 I=4,59
  500 FAL(I) = DLOG(DBLE(I-3)) + FAL(I-1)
  510 CONTINUE
C     REACTION SPECIFICATION
      READ (IR, 5) tit
C     (FMT 1X,79H)    TITLE CARD OF THE REACTION
      READ (IR,20) IN,IZ,KEYO
C     (FMT 3I4)       N, Z OF THE COMPOSITE NUCLEUS, KEY OF PROJECTILE
C                     N+Z = 0 --- TOP OF THE PROGRAM
      IAT = IN + IZ
      IF (IAT.LE.0) STOP
      IAC=IAT
      IZC=IZ
      A3=DBLE(IAT)**0.3333333
      READ(IR,30) EEXCO,ESTEP,SGR,AK
C     (FMT 3F8.)      EXC. ENERGY (MEV), EN. STEP (MEV), REACT. C. S. (MB
C                     SGR .LE. 0. --- SGR APPROXIMATED BY CHAGUG SUBROUTI
      READ(IR,21) B
C     (FMT 10F4.)     BINDING ENERGIES FOR NEUTRONS (NUCLEI ACCORDING
C                     THEIR KEYS (0,1,....,9), LATER FOR PROTONS (0-9)
      IEEXCO = IDINT(EEXCO/ESTEP+0.5)
      DO 520 I=1,10
      DO 520 J=1,2
  520 IB(I,J) = IDINT(B(I,J)/ESTEP+0.5)
      IEEXC = IEEXCO
      IEEXC1 = IEEXC
      AF = 2.*IAT / (IAT+1.)
      G = IAT / 13.
      GF=G*EF
      CO = 6.58195E-22*IAT**3. / (2.*PI*G*AK)
      C = CO*IEEXC*ESTEP
      C2 = .9536E14*ESTEP
      AKFC = 3.675E17*AF*ESTEP
      WRITE(IW,5) tit
C     INVERSE C.S. CALCULATION
      DO 540 I=1,3
      KEY=I
      IF (I.EQ.3) KEY=0
      DO 540 IE=1,68
      ENGY=DBLE(IE)*ESTEP
  540 SG(I,IE)=CHAGUG(ENGY)
      EGR=29.*DSQRT((1.+2./A3)/A3)
      KEY=KEYO
      CALL MASCHA
      MOO=IAO-1
      ATX=IAT-IAO
      IZX=IZ-IZO
      INX=IN-IAO+IZO
      DO 600 J=1,25
      R(1,J,1) = (DBLE(IAO-IZO) + (J-1)*INX/DBLE(IATX)) / (J+MOO)
      R(2,J,1) = (DBLE(  IZO  ) + (J-1)*IZX/DBLE(IATX)) / (J+MOO)
  600 CONTINUE
      JAV=MINO( IFIX( SNGL( DSQRT(0.299*G*IEEXC))), 20)
      DO 700 J=JAV,25
      R(1,J,1)= INX/DBLE(IATX)
  700 R(2,J,1)= IZX/DBLE(IATX)
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      IE = IEEXC - IB(1,1)
```

```
      IF (SGR.LE.0.) SGR=CHAGUG(ESTEP*IE)
      WRITE(IW,11) IAT,EEXCO,ESTEP,SGR,G,AK,C,EGR,B
      DO 800 J=1,2
      DO 800 IP=2,10
      DO 800 I=1,25
  800 R(J,I,IP) = 0.
C     THE MAXIMUM EXCITATION ENERGIES FOR A GIVEN CHAIN OF NUCLEI ARE
C     ESTABLISHED
      IXC(1) = IEEXCO - IB(1,1)
      IXC(2) = IEEXCO - IB(1,2)
      IXC(3) = IXC(1) - IB(2,1)
      IXC(4) = IXC(1) - IB(2,2)
      IXC(5) = IXC(2) - IB(3,2)
      IXC(6) = IXC(3) - IB(4,1)
      IXC(7) = IXC(3) - IB(4,2)
      IXC(8) = IXC(5) - IB(6,1)
      IXC(9) = IXC(5) - IB(6,2)
      IIIIIO = 0
 1000 IIIIIP = IIIIIO+1
      IF (IIIIIO-6) 1010,1005,1005
 1005 IIIIIA = 3
      GOTO 1035
 1010 IF (IIIIIO-3) 1020,1015,1015
 1015 IIIIIA = 2
      GOTO 1035
 1020 IF (IIIIIO-1) 1030,1025,1025
 1025 IIIIIA = 1
      GOTO 1035
 1030 IIIIIA = 0
 1035 CONTINUE
C     DENSITIES AND TRANSITION RATES CALCULATION
C     CYCLE OVER EXCITON NUMBER
      write(*,1357) iiiiiO
 1357 format(' Cycle ',i3)
      DO 3050 I=1,25
      IH = I-1
      IP = I-IIIIIA
      IP = IP+MOO
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      IP1 = IP+1
      IF (IIIIIO.EQ.0) GOTO 1050
      IEEXC1 = IXC (IIIIIO)
      IEEXC = IEEXC1
 1050 IF (IEEXC.LE.1) GOTO 4778
      N = IP+IH
      A0 = 0.25*(IP*IP+IH*IH+IP-3*IH)
      A1 = 0.25*((IP-1)**2+(IH-1)**2+IP-3*IH+2)
      A2 = 0.25*((IP+1)**2+(IH+1)**2+IP-3*IH-2)
      A3 = 0.5 *((IP+2)*IP1+IH*(IH+1))
      IF (IP.LE.0) GOTO 1250
      IF (IIIIIO.EQ.1) GOTO 1160
      IF (IIIIIO.EQ.3) GOTO 1180
      IF (IIIIIO.EQ.6) GOTO 1200
      GOTO 1250
C     R-FACTOR CALCULATION FOR SUBSEQUENT NUCLEI
 1160 CONTINUE
      R(1,I,2) = DMAX1 ((IP1*R(1,I,1) -1.DO)/DBLE(IP), 0.DO)
      R(2,I,2) = 1.DO - R(1,I,2)
      R(1,I,3) = DMIN1 (IP1*R(1,I,1)/DBLE(IP), 1.DO)
      R(2,I,3) = 1.DO - R(1,I,3)
      GOTO 1250
```

```
 1180 R(1,I,4) = DMAX1 ((IP1*R(1,I,2) -1.D0)/DBLE(IP), 0.D0)
      R(2,I,4) = 1.D0 - R(1,I,4)
      R(1,I,5) = DMAX1 ((IP1*R(1,I,3) -1.D0)/DBLE(IP), 0.D0)
      R(2,I,5) = 1.D0 - R(1,I,5)
      R(2,I,6) = 1.D0 - R(1,I,6)
      R(1,I,6) = DMIN1 (IP1*R(1,I,3)/DBLE(IP), 1.D0)
      GOTO 1250
 1200 R(1,I,7) = DMAX1 ((IP1*R(1,I,4) -1.D0)/DBLE(IP), 0.D0)
      R(2,I,7) = 1.D0 - R(1,I,7)
      R(1,I,8) = DMAX1 ((IP1*R(1,I,5) -1.D0)/DBLE(IP), 0.D0)
      R(2,I,8) = 1.D0 - R(1,I,8)
      R(1,I,9) = DMAX1 ((IP1*R(1,I,6) -1.D0)/DBLE(IP), 0.D0)
      R(2,I,9) = 1.D0 - R(1,I,9)
      R(1,I,10)= DMIN1 (IP1*R(1,I,6)/DBLE(IP), 1.D0)
      R(2,I,10)= 1.D0 - R(1,I,10)
C     ENERGY CYCLE
 1250 DO 3050 IE=1,IEEXC1
      E = IE*ESTEP
      IF (N.LE.0) GOTO 1270
      EP = E/ DBLE(N)
      EM = E/ DBLE(N+2)
      IF (EP.LE.2.) CP = DSQRT(7./EP)*DSQRT(2./EP)
      IF (EM.LE.2.) CM = DSQRT(7./EM)*DSQRT(2./EM)
      IF (EP.GE.2..AND.EP.LT.7.) CP = DSQRT(7./EP)
      IF (EM.GE.2..AND.EM.LT.7.) CM = DSQRT(7./EM)
      IF (EP.GE.7..AND.EP.LE.15.) CP = 1.
      IF (EM.GE.7..AND.EM.LE.15.) CM = 1.
      IF (EP.GT.15.) CP = DSQRT(EP/15.)
      IF (EM.GT.15.) CM = DSQRT(EM/15.)
      CP = C0*CP*EP
      CM = C0*CM*EM
 1270 TAU(I,IE) = 0.
      ALP(I,IE) = 0.
      ALM(I,IE) = 0.
      T1 (I,IE) = 0.
      EMG(I,IE)=0.
      EMP(I,IE)=0.
      IF (IIIIIO) 1350,1350,1300
 1300 TO(I,IE) = T2(IIIIIO,I,IE)
      GOTO 1450
 1350 TO(I,IE) = .
      DO 1400 J=1,5
 1400 T2(J,I,IE) = 0.
C     DENSITY AND TRANSITION RATES CALCULATION
 1450 OM(I,IE) = RO (E,G,IP,IH)
      IF (N.LE.0) GOTO 3050
      OMR(I,IE) = RO(E,G,IP-1,IH)
      GE = G*E
      HLP3 = 0.
      IF (GE-A1-GF.GE..01) HLP3 = (IH-1)*((GE-A1-GF)/(GE-A1)) ** (N-3)
      ALM(I,IE) = 0.5*IP*IH*(N-2)*(1.-HLP3)/CM
      IF (GE.LT.A3) GOTO 3050
      HLP3 = 0.
      IF (GE-A2-GF.GE..01) HLP3 = (IH+1) * DEXP ((N+1)*DLOG(GE-A2-GF)
     1                                          -(N-1)*DLOG(GE-A0))
      ALP(I,IE) = 0.5 * (DEXP((N+1)*DLOG(GE-A2)-(N-1)*DLOG(GE-A0)) -
     1                   HLP3) / (CP*(N+1))
C     END OF DENSITIES AND TRANSITION RATES
 3050 CONTINUE
      DO 3100 IE=1,IEEXC
      ALM( 1,IE) = 0.
      ALP(25,IE) = 0.
```

```
      DO 3100 I=1,3
 3100 SE(I,IE) = 0.
 3170 NN = 25
      DO 3200 I=4,25
      IF (ALP(I,IEEXC).NE.0.) GOTO 3200
      IF (I.LE.NN) NN=I
 3200 CONTINUE
C     EMISSION RATES CALCULATIONS FOR GIVEN NUCLEI
      DO 3500 I=1,NN
      IP = I-IIIIIA
      IP = IP+MOO
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      IH = I-1
      N = IP+IH
      IF (N.LE.0) GOTO 3500
C     ENERGY CYCLE
      DO 3480 IE = 1,IEEXC
      RO1 = OM(I,IE)
      IF (RO1.EQ.0.) GOTO 3480
      DO 3400 J=1,2
      T11 = 0.
      IEOM = IE -IB(IIIIIP,J)
      IEOM1 = IEOM-1
      IF (IEOM1.LE.0) GOTO 3400
      DO 3350 IEO=1,IEOM1
      IER = IEOM-IEO
      RO2 = OMR(I,IER)
      T11 = T11+SG(J,IEO)*IEO*RO2*ESTEP
 3350 CONTINUE
 3400 TAU(I,IE) = TAU(I,IE) + AKFC*R(J,I,IIIIIP)*T11
      T11=0.
      IF (IE.EQ.1) GOTO 3460
      IE1=IE-1
      DO 3450 IGM=1,IE1
      EGM = IGM*ESTEP
      IER = IE-IGM
      SGI = EGM*EGM*SG(3,IGM)
      T11 = T11 + N*SGI*OM(I,IER) / (N+G*EGM)
      IF (I    .NE.1) T11 = T11 + EGM*G*SGI*OM(I-1,IER)/((N-2)+G*EGM)
 3450 CONTINUE
 3460 EMP(I,IE)=TAU(I,IE)/RO1
      EMG(I,IE)=T11*C2/RO1
      T11=EMP(I,IE)+EMG(I,IE)+ALP(I,IE)+ALM(I,IE)
      IF (T11.NE.0.) TAU(I,IE) = 1. / T11
 3470 CONTINUE
 3480 CONTINUE
 3500 CONTINUE
C     END OF EMISSION RATES CALCULATIONS
C     IEE2 = (IEEXC-1)/2
C     IE = 2
C3600 WRITE(IW,20) IIIIIO,IE
C     DO 3650 I=1,NN
C     IJ = I-1
C     IF (TAU(I,IE).NE.0.) T11 = 1. / TAU(I,IE)
C     T111 = ALP(I,IE) + ALM(I,IE)
C     IF (OM(I,IE).NE.0.) WRITE IW,60) IJ,ALP(I,IE),ALM I,IE),T111,T11
C     IF DESIRED, OUTPUT OF INTRANUCLEAR TRANSITION RATES
C3650 CONTINUE
C     IF (IE-IEEXC) 3700,3750,3750
C3700 IE = IE+IEE2
C     IE = MIN0(IE,IEEXC)
C     GOTO 3600
```

```
C3750 WRITE(IW,15)
C     STARTING APPROXIMATION FOR MASTER EQUATIONS ITERATIONS
      IF (IIIIIO.NE.0) GOTO 4000
      NN1 = NN-1
      DO 3950 I=1,NN1
      P = 1.
      IF (I.EQ.1) GOTO 3850
      I1=I-1
      DO 3800 J=1,I1
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
 3800 P = P*TAU(J,IEEXC)*ALP(J,IEEXC)
 3850 TO(I,IEEXC) = TAU(I,IEEXC)*P * (1. + TAU(I,IEEXC)*ALP(I,IEEXC)
     1                                   *ALM(I+1,IEEXC)*TAU(I+1,IEEXC))
C     WRITE(IW,52) I,IEEXC,TAU(I,IEEXC),P,TO(I IEEXC)
 3950 CONTINUE
      GOTO 4050
 4000 DO 4030 I=1,25
      DO 4030 IE=1,IEEXC
 4030 TO(I,IE) = TO(I,IE)*TAU(I,IE)
 4050 CONTINUE
      WRITE(IW,15)
C     WRITE(IW,90) (TO(I,IEEXC) I=1,15)
      ITERMX = 20
      IF (IIIIIO.GE.3) ITERMX = 2
C
C     MASTER EQ. ITERATION FOR ONE NUCLEUS WITHIN THE CHAIN
C
      FEEDO = 1.
      FEED1 = 0.
      DO 4300 IEO=1,IEEXC
      IE = IEEXC+1-IEO
      IF (IE.NE.IEEXC) FEEDO = 0.
      IF (IIIIIO.EQ.0) GOTO 4080
      FEEDO = 0.
      DO 4070 I=1,NN
 4070 FEEDO = FEEDO+T2(IIIIIO,I,IE)
 4080 FEED  = FEEDO + FEED1
      IF (FEED.NE.0.) GOTO 4100
      DO 4090 I=1,NN
 4090 TO(I,IE)=0.
      GOTO 460
 4100 DO 450 ITER=1,ITERMX
      DO 400 I=1,NN
      IH = I-1
      IP = I-IIIIIA
      IP = IP+MOO
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      N = IP + IH
      T11 = 0.
      IF (N.LE.0.OR.OM(I,IE).EQ.0.) GOTO 400
      IF (I.NE.1) T11 = TO(I-1,IE)*ALP(I-1,IE)
      IF (I.NE.25) T11 = T11 + TO(I+1,IE)*ALM(I+1,IE)
      IF (IIIIIO.NE.0) T11 = T11 + T2(IIIIIO,I,IE)
      IF (IIIIIO.EQ.0.AND.I.EQ.1.AND.IE.EQ.IEEXC) T11 = T11 + 1.
C * * * STARTING CONFIGURATION WITH PO=A(PROJ), HO=0 * * * * * * * * * *
      T1111 = 0.
 4150 IF (IE.EQ.IEEXC) GOTO 4250
      IO = I
      IEO = IE
      CALL GAMMAS
 4250 T11 = T11 + T1111
      IF (T11.LE.1.D-38) T11=0.
```

```
  400 T1(I,IE) = T11*TAU(I,IE)
      DO 410 I=1,NN
  410 TO(I,IE) = T1(I,IE)
  415 IF (ITER.NE.ITERMX .AND. ITER.NE.1) GOTO 450
      IF (FEED.EQ.0.) GOTO 450
      OMT = 0.
      EMTG=0.
      EMTP=0.
      EMT = 0.
      DO 4620 I=1,NN
      OMT = OMT + OM(I,IE)
      EMTP=EMTP+TO(I,IE)*EMP(I,IE)
      EMTG=EMTG+TO(I,IE)*EMG(I,IE)
      EMT=EMTP+EMTG
 4620 CONTINUE
      IF (OMT.LE.0..OR.ITER.NE.1) GOTO 4690
      EMTOT = 0.
      DO 4630 I=1,NN
      T111 = 0.
      IF (TAU(I,IE).NE.0.) T111 = 1. / TAU(I,IE)
 4630 EMTOT = EMTOT + OM(I,IE) * (T111-AM(I,IE)-ALP(I,IE)) / OMT
      IF (EMTOT.NE.0.) EMTOT = (FEED-EMT) / EMTOT
      DO 4640 I=1,NN
 4640 TO(I,IE) = TO(I,IE) + EMTOT*OM(I,IE)/OMT
      IF (ITER.NE.ITERMX) GOTO 450
 4690 WRITE(IW,51) IIIIIO,ITER,IE,EMTP,EMTG,EMT,(TO(I,IE),I=1,6)
C     OUTPUT: NUCLEUS INDEX, NO. OF ITERATIONS, NO. OF ENERGY STEPS,
C             PARTICLE, GAMMA AND TOTAL EMISSION, TIME INTEGRALS OF THE
C             EXCITON STATES (N=1-17*)
  450 CONTINUE
  460 CONTINUE
      FEED1 = 0.
      IF (IE.EQ.1) GOTO 4300
      IE = IE-1
      DO 470 I=1,NN
      N = 2*I-IIIIIA-1
      N = N + MOO
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      T1111 = 0.
      IF (N.LE.0.OR.OM(I,IE).EQ.0.) GOTO 470
      IO = I
      IEO = IE
      CALL GAMMAS
  470 FEED1 = FEED1 + T1111
 4300 CONTINUE
C
C     MASTER EQ. ITERATION FINISHED
C
 4700 CONTINUE
      WRITE(IW,15)
C     NEUTRON, PROTON AND GAMMA SPECTRA CALCULATION
C
      write(iw,70)
      DO 5400 IE=2,IEEXC
      DO 5400 I=1,NN
      TOO = TO(I,IE)
      RO1= OM(I,IE)
      IF (RO1.EQ.0. .OR. TOO.EQ.0.) GOTO 5400
C     LOOP OVER N (J=1), P (J=2) AND GAMMA (J=3)
      DO 5380 J=1,3
      IEOM = IE
      IF (J-2) 5000,5000,5100
```

```
 5000 IEOM = IEOM-IB(IIIIIP,J)
      IF (IEOM.LE.1) GOTO 5380
 5100 IEOM1 = IEOM - 1
      N = 2*I-IIIIIA-1
      N = N + MOO
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      IF (N.LE.0) GOTO 5380
      DO 5350 IEO=1,IEOM1
      IER = IEOM - IEO
      EEO = ESTEP*IEO
      T11 = 0.
      IF (J.EQ.3) GOTO 5200
      T11 = SG(J,IEO)*EEO*OMR(I,IER)*R(J,I,IIIIIP)*AKFC
      GOTO 5300
 5200 SGI = EEO*EEO*SG(3,IEO)*C2
      T11 = SGI*N*OM(I,IER) / (N+G*EEO)
      IF (I.NE.1) T11 = T11 + EEO*G*SGI*OM(I-1,IER) / ((N-2)+G*EEO)
 5300 T11 = T11*TOO/RO1
      SE (J,IEO) = SE(J,IEO) + T11*SGR/ESTEP
      IF (IIIIIO.GE.3) GOTO 5350
      IIIIII = IIIIIO + IIIIIA + J
      IF (J.LE.2) T2(IIIIII,I,IER) = T2(IIIIII,I,IER) + T11
 5350 CONTINUE
 5380 CONTINUE
 5400 CONTINUE
C     SPECTRA OUTPUT
      DO 5500 IEO = 1,IEEXC
      EEO = ESTEP*IEO
      IF (IEO.EQ.IEEXC) GOTO 5450
      DO 5420 J=1,3
 5420 SE(J,IEEXC) = SE(J,IEEXC) + SE(J,IEO)*ESTEP
 5450 CONTINUE
      IF (IEO.NE.IEEXC) WRITE(IW,71) EEO, (SE(J,IEO),J=1,3)
      IF (IEO.EQ.IEEXC) WRITE(IW,72)      (SE(J,IEO),J=1,3)
 5500 CONTINUE
 4778 CONTINUE
C     NEXT NUCLEUS
      WRITE(IW,15)
      IIIIIO = IIIIIP
      IF (IIIIIO.LE.5) GOTO 1000
      GOTO 510
C
C     FORMATS
    4 FORMAT(1H1)
    5 FORMAT(1X,a70)
   11 FORMAT(' ATARG=',I3,'   EEXC=',F5.2,'   EN.STEP=',F6.3,'   SGR='
     1       ,F6.1, '   G=', F5.2/'   K=',F6.0,'   C=',E10.3,'   EGR=',
     2       F6.2///' KEY     0     1     2     3     4     5     6',
     3       '     7     8     9'/' B(N)',10F6.1/' B(P)',10F6.1/
     4       ' Akkermans and Gruppelaar approach, PC v. 10.01.1989'///)
   15 FORMAT(//1H )
   20 FORMAT(20I4)
   21 FORMAT(10F4.1)
   30 FORMAT(8F8.1)
   40 FORMAT(2F8.6)
   50 FORMAT(1X,I2,I4,I3,G11.4,1X,10G11.4)
   51 FORMAT(1X,I2,2I3,3F9.6/9X,6E10.3)
   52 FORMAT(1X,2I6,3G15.5)
   60 FORMAT(1X,I2,4E13.4)
   70 FORMAT(//' SPECTRA'//'  E (MeV)          neutrons        proton'
     1       's          gammas'/)
   71 FORMAT(1X,F8.3,3X,3G15.5)
```

```
   72 FORMAT(' Integral     ',3G15.5)
   90 FORMAT(1X,11G12.4)
      END
      FUNCTION RO (E, G, P, H)
C     EXCITON LEVEL DENSITY, CORRECTED FOR FINITE DEPTH OF NUCL. POT.
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON FAL(59),EF,IAC,IZC
      INTEGER P,H
      R = 0.
      GE = G*E
      AL = 0.5 * (P*(P+1) + H*(H-1))
      IF (GE.LT.AL) GOTO 1
      A = 0.25 * (P*P + H*H + P -3*H)
      GE = GE - A
      N = P + H
      IF (N.LE.0) GOTO 1
      CLFA = FAL(P+3) + FAL(H+3) + FAL(N+2)
      R = DEXP ((N-1)*DLOG(GE)-CLFA)
      IF (G*E-AL.LE.G*EF) GOTO 2
      R = R - H * DEXP ((N-1)*DLOG(GE-G*EF)-CLFA)
    2 R = G * R
    1 RO = R
      RETURN
      END
      SUBROUTINE GAMMAS
C     GAMMA EMISSION CALCULATION
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /GAM/ TO(25,68), OM(25,68), SG(3,68),AF,C2,ESTEP,G,T1111,
     1             IO, IAT, IEEXC, IEO, IZ, N
      IE = IEO
      I = IO
      IE1 = IE+1
      DO 10 IEG=IE1,IEEXC
      IF (OM(I,IEG).EQ.0.) GOTO 10
      IGM = IEG-IE
      GM = ESTEP*IGM
      SGI = GM*GM*SG(3,IGM) / (N+G*GM)
      T1111 = T1111 + TO(I,IEG)*SGI*N / OM(I,IEG)
      IF (I.EQ.25) GOTO 10
      IF (OM(I+1,IEG).NE.0.) T1111 = T1111 + TO(I+1,IEG)*GM*G*SGI
     1                                     / OM(I+1,IEG)
   10 CONTINUE
      T1111 = T1111*OM(I,IE)*C2
      RETURN
      END
      DOUBLE PRECISION FUNCTION CHAGUG (ENG)
      IMPLICIT REAL*8 (A-H, O-Z)
      COMMON FAL(59), EF, IAC, IZC
      COMMON /MC/ IAO,IZO,KEY
C     PARTICLE CROSS SECTION APPROXIMATION ACCORDING TO
C                            A. CHATTERJEE, K.H.N. MURTHY, S.K. GUPTA
C                                           PRAMANA 16 (1981), 391
C                                           NUCL. PHYS. SOL. ST. PHYS.
C                                                       SYMP. DELHI 1980
C                                           PRIVATE COMM. (FEB. 1981)
C       GAMMA  CROSS SECTION APPROXIMATED BY G.D.R. FORM,
C                            S.A. FAYANS (LECTURE, DUBNA, FEB. 1982)
C     KEY NUMBERS
C     0-GAMMA,   1-N,    2-P,    3-D,    4-T,    5-HE-3,    6-ALPHA
C     EN IS THE LABORATORY ENERGY IN MEV
C     THE RESULTING CROSS SECTION IS IN MB.
```

```
C     ******************************************************************
      EN=ENG
      CALL MASCHA
      A = DBLE(IAC-IAO)
      Z = DBLE(IZC-IZO)
      A3 = A**0.3333333
      IF (IAO.EQ.0) GOTO 3000
      A23= A3*A3
      DEL=0.
      IF (KEY.GE.3) DEL=1.2
      EC = 1.44*IZO*Z / (1.5*A3+DEL)
      EC2= EC*EC
      XI = DMAX1(EN,EC)
      EM=DMIN1(EN,61.D0)
      GOTO (100, 200, 300, 400, 500, 600), KEY
  100 CONTINUE
C     NEUTRONS
      P  =0.
      ALA=31.05/A3-25.91
      AMU=342.4*A3+21.89*A23
      ANU=0.223*A23*A23+0.673*A23+617.4
      EO =0.
      GOTO 2000
  200 CONTINUE
C     PROTONS
      P  =82.12/EC+2.39*A23/EC
      ALA=-0.521*A23-3.43
      AMU=150.2*A**0.59+946.3*(A-2.*Z)/A
      ANU=A23*(-43.9-76.25*EC)
      GOTO 1000
  300 CONTINUE
C     DEUTERONS
      P  =-38.21 + 922.6/EC - 2804./EC2
      ALA=-0.0323 *A - 5.48
      AM =A**0.48
      AMU=336.1*AM
      ANU= AM * ( 524.3 - 371.8*EC + 5.924*EC2)
      GOTO 1000
  400 CONTINUE
C     TRITONS
      P  =-11.04 + 619.1/EC - 2147./EC2
      ALA=-0.0426 *A -10.33
      AM =A**0.37
      AMU=601.9*AM
      ANU= AM * ( 583.0 - 546.2*EC + 1.718*EC2)
      GOTO 1000
  500 CONTINUE
C     HELIUM-3
      P  = -3.06 + 278.5/EC - 1389./EC2
      ALA=-0.00535*A -11.16
      AM =A**0.40
      AMU=555.5*AM
      ANU= AM * ( 687.4 - 476.3*EC + 0.509*EC2)
      GOTO 1000
  600 CONTINUE
C     ALPHAS
      P  = 10.95 - 85.2/EC + 1146./EC2
      ALA= 0.0643 *A -13.96
      AM =A**0.29
      AMU=781.2*AM
      ANU= AM * (-304.7 - 470.0*EC - 8.580*EC2)
```

```
 1000 Q = ALA-ANU/EC2-2.*P*EC
      R = AMU+2.*ANU/EC+P*EC2
      D = Q*Q-4.*R*P
      IF (D) 1100,1100,1200
 1100 EO= 0.
      GOTO 2000
 1200 D = DSQRT(D)
      E1= (-Q+D)/(2.*P)
      E2= (-Q-D)/(2.*P)
      IF (P.LT.0.) EO=DMIN1(E1,E2)
      IF (P.GE.0.) EO=DMAX1(E1,E2)
 2000 SIG = P*(EN-XI)**2 + ALA*EM + AMU + ANU*(2.D0-EN/XI)/XI
      IF (EN.LT.EO) SIG=0.
 2500 CHAGUG=SIG
      RETURN
 3000 CONTINUE
C     GAMMAS
      EGR=29.*DSQRT((1.D0+2.D0/A3)/A3)
      GAM=5.
      SGM=53.2*DBLE((IAC-IZC)*IZC)/DBLE(IAC)
      SIG=SGM * GAM*EN*EN/ ((EN*EN-EGR*EGR)**2+(GAM*EN)**2)
      GOTO 2500
    6 format(1x,a30)
      END
      SUBROUTINE MASCHA
C     MASS AND CHARGE SELECTION ACCORDING TO THE KEY
      COMMON /MC/ IA, IZ, KEY
      IZ=1
      IF (KEY.GE.5) IZ=2
      IF (KEY.LE.1) IZ=0
      IA=KEY-IZ
      RETURN
      END
```

APPENDIX B

INPUT DATA FILE

```
 46Ti (n,p) at 14.8 MeV    TEST RUN Bratislava, data of 28.12.1988
  25  22   1
 23.6       0.5    -1.       65.
 8.913.2 8.8 7.011.3 7.4  7.   7.   7.   7.
10.510.4 8.2 7.0 6.912.3  7.   7.   7.   7.
```

46Ti (n,p) at 14.8 MeV TEST RUN Bratislava, data of 28.12.1988
ATARG= 47 EEXC=23.60 EN.STEP= .500 SGR=1303.5 G= 3.62
K= 65. C= .109E-17 EGR= 19.03

KEY	0	1	2	3	4	5	6	7	8	9
B(N)	8.9	13.2	8.8	7.0	11.3	7.4	7.0	7.0	7.0	7.0
B(P)	10.5	10.4	8.2	7.0	6.9	12.3	7.0	7.0	7.0	7.0

Akkermans and Gruppelaar approach, PC v. 10.01.1989

0 20 47	1.043068	.001450	1.044518			
	.773E-21	.320E-21	.544E-21	.277E-20	.819E-20	.832E-20
0 20 46	.000000	.000000	.000000			
	.633E-31	.739E-31	.223E-29	.274E-28	.885E-28	.889E-28
0 20 2	.000000	.000465	.000465			
	.158E-14	.271E-14	.000E+00	.000E+00	.000E+00	.000E+00
0 20 1	.000000	.000000	.000000			
	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

SPECTRA

E (MeV)	neutrons	protons	gammas
.500	193.50	.00000	1.3575
1.000	228.36	.00000	1.1462
1.500	237.12	.00000	.93992
2.000	230.09	.00000	.78759
2.500	214.30	.36513	.64242
3.000	194.39	1.2626	.50272
3.500	173.29	2.2229	.37582
4.000	152.78	3.1621	.27014
4.500	133.83	4.0279	.18879
5.000	116.89	4.7970	.13090
5.500	102.12	5.4652	.92328E-01
6.000	89.403	5.9427	.67977E-01
6.500	78.556	6.0841	.53014E-01
7.000	69.338	6.0172	.44092E-01
7.500	61.491	5.8190	.39075E-01
8.000	54.756	5.5382	.36522E-01
8.500	48.941	5.2011	.35534E-01
9.000	43.816	4.8181	.35392E-01
9.500	39.217	4.3992	.35753E-01
10.000	34.999	3.9383	.36622E-01
10.500	31.038	3.4325	.37518E-01
11.000	27.255	2.8756	.38546E-01
11.500	23.553	2.2642	.39835E-01
12.000	19.869	1.5795	.41528E-01
12.500	16.146	.83665	.43824E-01
13.000	12.345	.00000	.46940E-01
13.500	8.3866	.00000	.51167E-01
14.000	4.3145	.00000	.56886E-01
14.500	.00000	.00000	.64603E-01
15.000	.00000	.00000	.74963E-01
15.500	.00000	.00000	.88888E-01
16.000	.00000	.00000	.10740
16.500	.00000	.00000	.13159
17.000	.00000	.00000	.16214
17.500	.00000	.00000	.19814

18.000	.00000	.00000	.23540
18.500	.00000	.00000	.26572
19.000	.00000	.00000	.27954
19.500	.00000	.00000	.27274
20.000	.00000	.00000	.24971
20.500	.00000	.00000	.21917
21.000	.00000	.00000	.18814
21.500	.00000	.00000	.16037
22.000	.00000	.00000	.13699
22.500	.00000	.00000	.11786
23.000	.00000	.00000	.10235
Integral	1320.1	40.025	5.1151

1 20 28 .070331 .045300 .115632
.000E+00 .117E-19 .674E-18 .576E-17 .112E-16 .542E-17

SPECTRA

E (MeV)	neutrons	protons	gammas
.500	160.26	.00000	994.00
1.000	.00000	.00000	946.81
1.500	.00000	.00000	831.76
2.000	.00000	.00000	751.34
2.500	.00000	17.869	677.99
3.000	.00000	14.110	608.68
3.500	.00000	.00000	541.39
4.000	.00000	.00000	476.11
4.500	.00000	.00000	413.75
5.000	.00000	.00000	354.96
5.500	.00000	.00000	300.56
6.000	.00000	.00000	251.14
6.500	.00000	.00000	207.05
7.000	.00000	.00000	168.34
7.500	.00000	.00000	134.88
8.000	.00000	.00000	106.36
8.500	.00000	.00000	82.309
9.000	.00000	.00000	62.401
9.500	.00000	.00000	46.222
10.000	.00000	.00000	33.342
10.500	.00000	.00000	23.291
11.000	.00000	.00000	15.608
11.500	.00000	.00000	9.9040
12.000	.00000	.00000	5.8327
12.500	.00000	.00000	3.0521
13.000	.00000	.00000	1.3176
13.500	.00000	.00000	.35579
14.000	.00000	.00000	.00000
Integral	80.128	15.989	4024.4

2 20 21 .000193 .000001 .000194
.000E+00 .309E-23 .112E-21 .550E-21 .548E-21 .911E-22

SPECTRA

E (MeV)	neutrons	protons	gammas