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ISOTOPES – A PROGRAM FOR NEUTRON PRODUCT YIELDS AND DECAY CALCULATIONS USING A CONTROL DATA 1604-A COMPUTER

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ISOTOPES DEVELOPMENT CENTER

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ABSTRACT

A computer program was developed to calculate the optimum time of neutron irradiation for maximum yield, the specific activity of the product isotope in curies per gram of target material, and the combined specific activity of the target and product isotopes for any general first-order reaction or decay problem. The program was written in the FORTRAN-63 language for the Control Data 1604-A computer.

INTRODUCTION

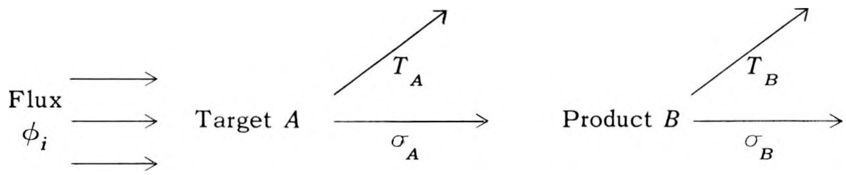
The optimum time of irradiation of a target in a reactor at a particular neutron flux, the resulting specific activity of the product, and the combined activity of product and target material are important in evaluating production methods for reactor-produced isotopes. A computer program was developed jointly by the ORNL Isotopes Division and Mathematics Division to handle these calculations. The program uses solutions to the "Bateman equations," and with it one can calculate product activity yields by either reaction or decay, allowing for burnup and decay of both target and product.

This program can be applied to other physical and chemical first-order reactions to solve for the time of maximum yield by adapting the existing symbols to fit the problem.

The derivation of the equations and explanation of the code with applications are discussed in this report.

THEORY

A general example of the reactor production of a radioisotope product isotope is the following:



A target material containing a natural or enriched abundance of a particular isotope is placed in a reactor with a neutron flux ϕ_i incident upon the material. The target A may be radioactive with a half-life T_A and have a total absorption cross section σ_A. The product isotope B may have a half-life T_B and a reaction cross section σ_B.

The differential equations describing the rate of change of the target isotope A and the product isotope B and the solutions to these equations are shown in the following:[1,2]

$$\frac{dN_A}{dt} = -(0.693^*/T_A + \phi_i\sigma_A)N_A \ , \tag{1}$$

$$N_A = N_0 \exp\left[-(0.693/T_A + \phi_i\sigma_A)t\right] \ ; \tag{2}$$

$$\frac{dN_B}{dt} = \phi_i\sigma_A N_A - (0.693/T_B + \phi_i\sigma_B)N_B \ , \tag{3}$$

$$N_B = \frac{\phi_i\sigma_A N_0}{(0.693/T_B + \phi_i\sigma_B) - (0.693/T_A + \phi_i\sigma_A)} \{\exp\left[-(0.693/T_A + \phi_i\sigma_A)t\right] - \exp\left[-(0.693/T_B + \phi_i\sigma_B)t\right]\} \ . \tag{4}$$

Optimum Time Formula

In order to find the value t for which the function $N_B(t)$ reaches a maximum, the derivative of the function with respect to t is set equal to zero.

$$\text{Let } r_A = (0.693/T_A + \phi_i\sigma_A) \ ,$$

$$r_B = (0.693/T_B + \phi_i\sigma_B) \ .$$

---

*Programmed 0.69315.

[1] R. D. Evans, *The Atomic Nucleus*, p. 477, McGraw-Hill, New York, 1955.

[2] M. P. Lietzke and H. C. Claiborne, *CRUNCH — An IBM 704 Code for Calculating N Successive First Order Reactions*, ORNL-2958 (Oct. 24, 1960).

Then

$$\frac{dN_B}{dt} = \frac{\phi_i \sigma_A}{r_B - r_A} [-r_A \exp(-r_A t_m) + r_B \exp(-r_B t_m)] = 0 .$$

Hence

$$\exp[(r_B - r_A)t_m] = r_B/r_A .$$

Substituting the values for r_A and r_B and taking the logarithm, the time for maximum yield t_m is

$$t_m = \frac{\ln\left(\frac{0.693/T_B + \phi_i \sigma_B}{0.693/T_A + \phi_i \sigma_A}\right)}{(0.693/T_B + \phi_i \sigma_B) - (0.693/T_A + \phi_i \sigma_A)} . \tag{5}$$

Equation (5) was used in the program to calculate the time for maximum yield using a particular flux ϕ_i.

Product Activity

The equation describing the activity, ACT, of the product isotope follows from the solution in Eq. (4). Activity in disintegrations per second for N_B is

$$\text{ACT (dis/sec)} = \frac{0.693}{T_B} N_B . \tag{6}$$

In order to convert the relation into curies per gram of target material when the target isotope has an isotopic abundance I (decimal fraction), it is necessary to transform the equation in the following manner.

Let

I = isotopic abundance (or enrichment) of target isotope in the target material,
$A = 6.0248 \times 10^{23}$ atoms/mole (Avogadro's number), and
W = weight in grams of one mole of the target material;

then

$$\left(\frac{\text{initial number of atoms of isotope } A}{\text{grams of target material}}\right) = N_o = \frac{IA}{W} . \tag{7}$$

In order to convert from disintegrations per gram of target material to curies per gram,

$$\text{ACT (curies/g)} = \frac{1}{3.700 \times 10^{10} \text{ dis/curie}} \frac{IA}{W} \frac{0.693}{T_B} N_B . \tag{8}$$

Hence the equation for radioactivity of the product isotope B from Eqs. (4), (5), and (8) is

$$\text{ACT (curies/g)} = \frac{1.128 \times 10^{13}\,(I/W\,T_B)\,\phi_i\sigma_A}{0.693/T_B + \phi_i\sigma_B - 0.693/T_A - \phi_i\sigma_A}\,\{\exp\,[-(0.693/T_A + \phi_i\sigma_A)t_m]$$

$$- \exp\,[-(0.693/T_B + \phi_i\sigma_B)t_m]\}\,. \quad (9)$$

Finally the combined radioactivity of the target isotope, if any, and the radioactivity of the product isotope is

$$\text{ACT}_{(\text{combined})} = \frac{1.128 \times 10^{13}}{T_A\,W}\,I\,\exp\,[-(0.693/T_A + \phi_i\sigma_A)t_m] + \text{ACT}_{(B)}\,. \quad (10)$$

In this program, $\text{ACT}_{(\text{combined})}$ and $\text{ACT}_{(B)}$ are calculated using Eqs. (9) and (10).

DESCRIPTION OF PROGRAM

Program ISOTOPES is written entirely in the FORTRAN-63 language and requires no subroutines other than those supplied with the calling program. The program contains two options that enable it to be used in different ways:

1. Normally the program performs the computations for a reaction involving a target and a product at various flux values. The computations may be performed for a simple decay involving a parent and daughter as described below.
2. The program can also perform the computations for maximum yield at a given arbitrary time.

Input

The input data are entered on cards. In order to describe the input, the cards are divided into two groups. The cards of the first group are described in Table 1 and supply the number of fluxes to be considered and their values. A minimum of 2 and a maximum of 100 values may be used. Each reaction or decay for which the computations are to be done requires the two cards described in Table 2. These cards supply information about each isotope. The cards representing all the reactions or decays being considered make up the second group. The cards of the first group precede those of the second in the data package.

It should be noted that the half-lives of the isotopes may be entered with units in seconds, minutes, hours, days, or years. This will facilitate their entry directly from most tables of half-lives without the need of converting to a uniform unit of time.

To use the options mentioned above, the following entries should be made on card 1 of Table 2:

1. To designate the type of process taking place, enter in column 65
   - *a.* target-product reaction – 0 or blank;
   - *b.* simple decay – 1.

2. To introduce an arbitrary time for maximum yield instead of computing it, enter the desired time[3] in columns 51–60. For convenience in reading the output, enter an asterisk in column 8 of both card 1 and card 2 of Table 2. At all other times columns 8 and 51–60 must be blank.

Output

The output consists of the input parameters followed by the results of the calculations for TMAX (time for maximum yield in days), PRODUCT ACT (activity of the product or daughter isotope in curies/gram), and COMBINED ACT (combined activity of the target and product isotopes or the parent and daughter isotopes). If the input parameters are such that no time for maximum yield is computed, the letters NO MAX will be printed for time, product activity, and combined activity.

ACKNOWLEDGMENT

The authors wish to thank J. J. Pinajian for his suggestions and encouragement in developing this program.

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[3]This time is entered in the same manner as the half-lives of the isotopes.

Table 1. Input Data.[a] Flux Values

Card No.	Field[b]	Variable	Type	Description
1	1–5	NUMPHI	INTEGER	Number of different neutron fluxes to be used (2 ≦ NUMPHI ≦ 100)
2	1–10	PHI(1)	FL. PT.	First flux value
	11–20	PHI(2)	FL. PT.	Second flux value
	21–30	PHI(3)	FL. PT.	Third flux value
	.	.	.	.
	.	.	.	.
	.	.	.	.
	71–80	PHI(8)	FL. PT.	Eighth flux value
2*a*	1–10	PHI(9)	FL. PT.	Ninth flux value
	.	.	.	Continuing in like manner for all values of PHI
	.	.	.	(number of "PHI-cards"
	.	.	.	is NUMPHI/8)

[a]Units on card No. 2 are neutrons cm^{-2} sec^{-1} while the values on card No. 1 are an integer value.
[b]All values are right-adjusted.

Table 2. Input Data. Isotope Values

Card No.	Field[a]	Variable	Type	Units	Description
1	1–7	ATOMA	BCD		Up to 7 alphanumeric characters giving the symbol and atomic number of the target or parent isotope
	8	*	BCD		Enter * only when an arbitrary time is introduced
	11–20	SIGMAA	FL. PT.	Barns	Reaction cross section of the target or parent
	21–30	TA	FL. PT.	Sec, min, hr, day, or year	Half-life of the target or parent. In column 30 enter whichever is appropriate: S ...... seconds M ...... minutes H ...... hours D ...... days Y ...... years
	31–40	ABUNA	FL. PT.	Decimal fraction ($\leq$ 1.0)	Relative abundance of the target or parent
	41–50	WTA	FL. PT.	Grams	Weight of one mole of the target or parent
	51–60	TMAXREAD	FL. PT.	Sec, min, hr, day, or year	Arbitrary time for maximum yield (blank if not desired); enter in like manner as entered for half-life
	65	OP	INTEGER		Type of process: target-product reaction — 0 or blank; simple decay — 1
2	1–7	ATOMB	BCD		Up to 7 alphanumeric characters giving the symbol and atomic number of the product isotope or daughter
	8	*	BCD		Enter * only when an arbitrary time is introduced
	11–20	SIGMAB	FL. PT.	Barns	Reaction cross section of the product or daughter
	21–30	TB	FL. PT.	Sec, min, hr, day, or year	Half-life of the product or daughter; column 30 is similar to that of TA above

[a]All values are right-adjusted.

APPENDIX A – SAMPLE PROBLEMS

Sample Problem 1

The problem of $^{121}Sb(n,\gamma)^{122}Sb$ illustrates a simple (n,γ) capture accompanied by product decay.

$$^{121}Sb \xrightarrow[\sigma_A = 6.8 \text{ barns}]{} {}^{122}Sb \nearrow T_B = 2.8 \text{ days}$$

$\phi = 2 \times 10^{14}$ neutrons cm^{-2} sec^{-1}

I (isotopic abundance of ^{121}Sb) = 0.5725

A (gram-atomic weight of natural Sb) = 121.75 g

The quantity TMAX is the optimum time of irradiation at the specified neutron flux necessary to produce a maximum amount of ^{122}Sb. The product specific activity of ^{122}Sb is calculated in curies per gram of starting (target) material (natural Sb). The combined activity (curies/g) is the activity of both ^{122}Sb and ^{121}Sb, which in this particular case is the same as the product activity. The following tabulation shows the input information:[4]

Isotope	Cross Section (barns)	Half-Life	I	Weight (g)	FLUX
SB 121	6.8	0.0 S	0.57250	121.750	2.0×10^{14}
SB 122	0.0	2.8 D			2.0×10^{14}

Note that the value 2×10^{14} is repeated because the program requires a minimum of two flux values. The value for the cross section of ^{122}Sb is not known and is therefore listed as zero.

This same information is written in the proper form and in the appropriate columns of a standard 650 data input sheet. See Fig. 1. The computer output is shown in Fig. 2.

For an arbitrary irradiation time, the isotope has an asterisk in column 8 of input and output, which indicates the calculation for specific activities of product and combined activity will be based upon that time rather than a TMAX value. For three arbitrary times of 7 days, 14 days, and 365 days, see Fig. 3.

---

[4]The half-life of a stable isotope is listed as zero in input data to the computer for convenience in programming.

650 DATA SHEET

REQUEST________ JOB TITLE________ WRITTEN BY________ DATE________

1 - 10	11 - 20	21 - 30	31 - 40	41 - 50	51 - 60	61 - 70	71 - 80
2							
2.0+14	2.0+14						
SB 121	6.8	05	0.57250	121.750			
SB 122	0	2.8D					

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Fig. 1. Input for Sample Problem 1.

ISOTOPE	CROSS SECTION (BARNS)	HALF-LIFE	OP	I	WEIGHT (GRAMS)	FLUX	TMAX (DAYS)	PRODUCT ACT (C/G)	COMBINED ACT (C/G)
SB 121	6.80000*+000	.00000*+000S	0	.57250	121.750	2.0000*+014	3.0929*+001	1.0369*+002	1.0369*+002
SB 122	.00000*+000	2.80000*+000D				2.0000*+014	3.0929*+001	1.0369*+002	1.0369*+002

Fig. 2. Output for Sample Problem 1. (TMAX calculations)

ISOTOPE	CROSS SECTION (BARNS)	HALF-LIFE	OP	I	WEIGHT (GRAMS)	FLUX	TMAX (DAYS)	PRODUCT ACT (C/G)	COMBINED ACT (C/G)
SB 121 *	6.80000*+000	.00000*+000S	0	.57250	121.750	2.0000*+014	7.0000*+000	8.5628*+001	8.5628*+001
SB 122 *	.00000*+000	2.80000*+000D				2.0000*+014	7.0000*+000	8.5628*+001	8.5628*+001
SB 121 *	6.80000*+000	.00000*+000S	0	.57250	121.750	2.0000*+014	1.4000*+001	1.0069*+002	1.0069*+002
SB 122 *	.00000*+000	2.80000*+000D				2.0000*+014	1.4000*+001	1.0069*+002	1.0069*+002
SB 121 *	6.80000*+000	.00000*+000S	0	.57250	121.750	2.0000*+014	3.6500*+002	9.9749*+001	9.9749*+001
SB 122 *	.00000*+000	2.80000*+000D				2.0000*+014	3.6500*+002	9.9749*+001	9.9749*+001

Fig. 3. Output for Sample Problem 1 with Arbitrary Irradiation Times.

Sample Problem 2

The following is an example of a simple decay problem. Consider the parent ^{131}Te producing ^{131}I by decay. The product is also radioactive.

$$^{131}\mathrm{Te} \xrightarrow[T_A = 30 \text{ hr}]{\beta^-} \quad ^{131}\mathrm{I} \xrightarrow[T_B = 8.05 \text{ days}]{\beta^-}$$

$\phi = 0$

$I = 0.1\%$

$A = 127.60$ g

The above information is shown on the input data sheet of Fig. 4. Results of the calculations are shown in the first two lines of the output in Fig. 5.

Sample Problem 3

This problem demonstrates the possibility of a target and a product both having a half-life due to both decay and neutron capture.

$$^{180}\mathrm{Aa} \xrightarrow[\sigma_A = 600 \text{ barns}]{} \ (\nearrow T_A = 5 \text{ years}) \quad ^{181}\mathrm{Bb} \xrightarrow[\sigma_B = 40 \text{ barns}]{} \ (\nearrow T_B = 26 \text{ days})$$

$\phi = 5.0 \times 10^{13}$, 1.0×10^{14}, 2.0×10^{14}

$I = 78.25\%$

$A = 180.00$ g

This problem also illustrates that the various half-lives may be entered in seconds (S), minutes (M), hours (H), days (D), or years (Y) by simply using the appropriate letter following the number. The results of the calculations for this problem are listed as the second case on the output in Fig. 5.

Sample Problems 4 and 5

These problems will show the zero activity and NO MAX characteristics of the program. In problem 4, the target and the product do not decay.

$$^{95}\mathrm{Mo} \xrightarrow[\sigma_A = 14 \text{ barns}]{} \quad ^{96}\mathrm{Mo} \xrightarrow[\sigma_B = 1 \text{ barn}]{}$$

$\phi = 3 \times 10^{15}$

$A = 95.94$ g

$I = 15.72\%$

650 DATA SHEET

REQUEST______ JOB TITLE______ WRITTEN BY______ DATE______

1 - 10	11 - 20	21 - 30	31 - 40	41 - 50	51 - 60	61 - 70	71 - 80
5							
5.0+13	1.0+14	2.0+14	3.0+15	1.0+15			
TE 131	0	30H	0.001	127.60		1	
I 131	0	8.05D					
AA 180	600	5Y	0.7825	180			
BB 181	40	26D					
MØ 95	14	0S	0.1572	95.94			
MØ 96	1	0S					
KK 50	135	1.0+3Y	0.224	49.998			
LL 51	0	0S					

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Fig. 4. Input for Sample Problems 2, 3, 4, and 5.

ISØTØPE	CRØSS SECTIØN (BARNS)	HALF-LIFE	ØP	I	WEIGHT (GRAMS)	FLUX	TMAX (DAYS)	PRØDUCT ACT (C/G)	CØMBINED ACT (C/G)
TE 131	.00000■+000	3.00000■*001H	1	.00100	127.500	---	3.9762■+000	9.0232■*001	1.8048■+002
I 131	.00000■+000	8.05000■*000D							
AA 180	6.00000■+002	5.00000■*000Y	0	.78250	180.000	5.0000■+013	9.2221■+001	1.6032■*003	1.8396■+003
BB 181	4.00000■+001	2.60000■*001D				1.0000■+014	7.3677■+001	2.7811■*003	2.9875■+003
						2.0000■+014	5.6255■+001	4.5203■*003	4.6902■+003
						3.0000■+015	1.2093■+001	1.3916■*004	1.3963■+004
						1.0000■+015	2.4901■+001	1.0237■*004	1.0322■+004
MØ 95	1.40000■+001	.00000■*000S	0	.15720	95.940	5.0000■+013	4.6992■+004	.0000■*000	.0000■+000
MØ 96	1.00000■+000	.00000■*000S				1.0000■+014	2.3495■+004	.0000■*000	.0000■+000
						2.0000■+014	1.1748■+004	.0000■*000	.0000■+000
						3.0000■+015	7.8320■+002	.0000■*000	.0000■+000
						1.0000■+015	2.3496■+003	.0000■*000	.0000■+000
KK 50	1.35000■+002	1.00000■*003Y	0	.22400	49.998	5.0000■+013	NØ MAX	NØ MAX	NØ MAX
LL 51	.00000■+000	.00000■*000S				1.0000■+014	NØ MAX	NØ MAX	NØ MAX
						2.0000■+014	NØ MAX	NØ MAX	NØ MAX
						3.0000■+015	NØ MAX	NØ MAX	NØ MAX
						1.0000■+015	NØ MAX	NØ MAX	NØ MAX

Fig. 5. Output for Sample Problems 2, 3, 4, and 5.

In problem 5 the target has both decay and a neutron capture cross section, but the product has neither.

$$^{50}\text{Kk} \xrightarrow[\sigma = 135 \text{ barns}]{} \qquad ^{51}\text{Ll}$$

$$\nearrow T_{1/2} = 10^3 \text{ years}$$

$\phi = 1 \times 10^{15}$

$A = 49.998\text{g}$

$I = 22.4\%$

Hence, there is no finite time for TMAX and no final activity value; so the program prints out NO MAX for all calculations. See the last case in the output in Fig. 5.

APPENDIX B – FORTRAN-63 CALLING PROGRAM

This section contains a listing of the FORTRAN-63 calling program and the subroutines associated with it. The FORTRAN or binary decks are available from the authors.

```
      PROGRAM ISOTOPES
      TYPE INTEGER BOOL,TESTA,TESTB,TESTT,UNITA,UNITB,UNITT
      TYPE INTEGER FMT,APE,VAR
      DIMENSIONPHI(100),FMT(10),APE(8),VAR(5),TIME(5),BOOL(5)
      COMMONFMT,VAR,APE,ATOMA,SIGMAA,TA,UNITA,ABUNA,WTA,TMAXREAD,ATOMB,
     1SIGMAB,TB,UNITB,TASTORE,TBSTORE,OP
      FMT(1)=8H(1HO,A8,
      FMT(2)=6HE14.5,
      FMT(3)=6HE14.5,
      FMT(4)=6HA1,I3,
      FMT(5)=6HF10.5,
      FMT(6)=5HF9.3,
      FMT(7)=6HE16.4,
      VAR(1)=8H(1H ,60X
      VAR(2)=7H(E15.4,
      APE(1)=8H(1H ,A8,
      APE(2)=6HE14.5,
      APE(3)=6HE14.5,
      APE(4)=7HA1,23X,
      APE(5)=6HE15.4,
      TIME(1)=1.0
      TIME(2)=60.0
```

```
      TIME(3)=3600.0
      TIME(4)=8.64E+4
      TIME(5)=3.1536E+7
      BOOL(1)=1HS                                                     SECONDS
      BOOL(2)=1HM                                                     MINUTES
      BOOL(3)=1HH                                                     HOURS
      BOOL(4)=1HD                                                     DAYS
      BOOL(5)=1HY                                                     YEARS
      M=0
      NUMOP=0
      LINE=0
  998 READ(50,100)NUMPHI
  100 FORMAT(I5)
      READ(50,111)(PHI(I),I=1,NUMPHI)
  111 FORMAT(8E10.0)
    2 READ(50,103)ATOMA,SIGMAA,TA,UNITA,ABUNA,WTA,TMAXREAD,UNITT,OP
      IF(SIGMAA+TA+ABUNA+WTA+TMAXREAD+FLOATF(OP))999,998,999
  999 READ(50,103)ATOMB,SIGMAB,TB,UNITB
  103 FORMAT(A8,2X,E10.0,E9.0,A1,2E10.0,E9.0,A1,I5)
      TASTORE=TA
      TBSTORE=TB
      IF(OP)91,36,91
   91 IF(SIGMAA)36,92,36
   92 IF(SIGMAB)36,35,36
   36 IF(NUMPHI-50)42,42,45
   42 M=M+1
   37 LINE=(NUMPHI+1)*M+3*NUMOP
      IF(LINE-51)40,40,47
   47 IF(OP)93,39,93
   93 IF(SIGMAA)39,94,39
   94 IF(SIGMAB)39,38,39
   39 M=1
      NUMOP=0
      LINE=NUMPHI+1
      GOTO45
   38 M=0
      NUMOP=1
      LINE=3
      GOTO45
   40 IF(M+NUMOP-2)45,90,90
   35 NUMOP=NUMOP+1
      GOTO37
   45 WRITE(51,101)
```

```
101 FORMAT(24H1ISOTOPE    CROSS SECTION,3X,9HHALF-LIFE,4X,2HOP,5X,1HI,
   16X,6HWEIGHT,9X,4HFLUX,11X,4HTMAX,7X,25HPRODUCT ACT  COMBINED ACT)
    WRITE(51,102)
102 FORMAT(1H ,13X,7H(BARNS),32X,7H(GRAMS),23X,6H(DAYS),2(9X,5H(C/G)))
 90 DO71I=1,5
    TESTA=(UNITA.AND.(.NOT.BOOL(I))).OR.((.NOT.UNITA).AND.BOOL(I))
    IF(TESTA)71,72
 71 CONTINUE
    WRITE(51,104)UNITA,ATOMA
104 FORMAT(1HO,A1,70H IS AN IMPROPER ENTRY FOR UNITS, MUST BE S, M, H,
   1 D OR Y.  ISOTOPE IS ,A7)
    GOTO2
 72 TA=TA*TIME(I)
    DO73J=1,5
    TESTB=(UNITB.AND.(.NOT.BOOL(J))).OR.((.NOT.UNITB).AND.BOOL(J))
    IF(TESTB)73,74
 73 CONTINUE
    WRITE(51,104)UNITB,ATOMB
    GOTO2
 74 TB=TB*TIME(J)
    IF(TMAXREAD)996,997,996
996 DO 995 J=1,5
    TESTT=(UNITT.AND.(.NOT.BOOL(J))).OR.((.NOT.UNITT).AND.BOOL(J))
    IF(TESTT)995,994
995 CONTINUE
    WRITE(51,104)UNITT,ATOMA
    GO TO 2
994 TMAXREAD=TMAXREAD*TIME(J)
997 IF(OP)86,87,86
 86 IF(SIGMAA)87,88,87
 88 IF(SIGMAB)87,89,87
 89 CALL OPTION
    GOTO2
 87 IF(TA)5,4,5
  5 IF(TB)6,9,6
  4 IF(TB)7,8,7
  6 DO29I=1,NUMPHI
    SIGMAB=SIGMAB*1.0E-24
    SIGMAA=SIGMAA*1.0E-24
    CALL YESMAX
    FACT1=0.69315/TA+PHI(I)*SIGMAA
    FACT2=0.69315/TB+PHI(I)*SIGMAB
    DENOM=FACT2-FACT1
    IF(DENOM)30,31,30
```

```
 30 IF(TMAXREAD)60,44,60
 44 TMAX=LOGF(FACT2/FACT1)/DENOM
    GOTO50
 60 TMAX=TMAXREAD
 50 IF(OP)80,81,80
 80 ACT1=7.81704E+12*ABUNA/(WTA*TB*TA)*(EXPF(-FACT1*TMAX)-EXPF(-FACT2*
   1TMAX))/DENOM
    GOTO82
 81 ACT1=1.128E+13*ABUNA*SIGMAA/(WTA*TB)*PHI(I)*(EXPF(-FACT1*TMAX)-
   1EXPF(-FACT2*TMAX))/DENOM
 82 ACT2=1.128E+13*ABUNA*EXPF(-FACT1*TMAX)/(TA*WTA)+ACT1
    TMAX=TMAX/8.64E+4
 59 SIGMAA=SIGMAA/1.0E-24
    SIGMAB=SIGMAB/1.0E-24
    IF(I-2)32,33,34
 32 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),TMAX,
   1ACT1,ACT2
    GOTO29
 33 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),TMAX,ACT1,ACT2
    GOTO29
 34 WRITE(51,VAR)PHI(I),TMAX,ACT1,ACT2
    GOTO29
 31 ITMAX=8HNO MAX
    IACT1=ITMAX
    IACT2=ITMAX
    CALL NOMAX
    SIGMAA=SIGMAA/1.0E-24
    SIGMAB=SIGMAB/1.0E-24
    IF(I-2)332,333,334
332 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),ITMAX,
   1IACT1,IACT2
    GO TO 29
333 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),ITMAX,IACT1,IACT2
    GO TO 29
334 WRITE(51,VAR)PHI(I),ITMAX,IACT1,IACT2
 29 CONTINUE
    GOTO2
  7 DO21I=1,NUMPHI
    SIGMAA=SIGMAA*1.0E-24
    SIGMAB=SIGMAB*1.0E-24
    IF(SIGMAA)65,22,65
 65 CALL YESMAX
    FACT1=0.69315/TB+PHI(I)*SIGMAB
    FACT2=PHI(I)*SIGMAA
```

```
      DENOM=FACT1-FACT2
      IF(DENOM)17,22,17
   17 IF(TMAXREAD)61,56,61
   56 TMAX=LOGF(FACT1/FACT2)/DENOM
      GOTO55
   61 TMAX=TMAXREAD
   55 IF(OP)84,83,84
   84 ACT1=0.0
      GOTO85
   83 ACT1=1.128E+13*ABUNA/(WTA*TB)*FACT2*(EXPF(-FACT2*TMAX)-EXPF(-FACT1
     1*TMAX))/DENOM
   85 ACT2=ACT1
      TMAX=TMAX/8.64E+4
   58 SIGMAA=SIGMAA/1.0E-24
      SIGMAB=SIGMAB/1.0E-24
      IF(I-2)18,19,20
   18 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),TMAX,
     1ACT1,ACT2
      GOTO21
   19 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),TMAX,ACT1,ACT2
      GOTO21
   20 WRITE(51,VAR)PHI(I),TMAX,ACT1,ACT2
      GOTO21
   22 ITMAX=8HNO MAX
      IACT1=ITMAX
      IACT2=ITMAX
      CALL NOMAX
      SIGMAA=SIGMAA/1.0E-24
      SIGMAB=SIGMAB/1.0E-24
      IF(I-2)318,319,320
  318 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),ITMAX,
     1IACT1,IACT2
      GO TO 21
  319 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),ITMAX,IACT1,IACT2
      GO TO 21
  320 WRITE(51,VAR)PHI(I),ITMAX,IACT1,IACT2
   21 CONTINUE
      GOTO2
    8 DO23I=1,NUMPHI
      SIGMAA=SIGMAA*1.0E-24
      SIGMAB=SIGMAB*1.0E-24
      IF(SIGMAB)99,25,99
   99 IF(SIGMAA)1,25,1
    1 FACT1=PHI(I)*SIGMAA
```

```
      FACT2=PHI(I)*SIGMAB
      CALL YESMAX
      DENOM=FACT2-FACT1
      IF(DENOM)24,25,24
   24 IF(TMAXREAD)62,51,62
   51 TMAX=LOGF(FACT2/FACT1)/DENOM
      GOTO52
   62 TMAX=TMAXREAD
   52 ACT1=0.0
      ACT2=0.0
      TMAX=TMAX/8.64E+4
   66 SIGMAA=SIGMAA/1.0E-24
      SIGMAB=SIGMAB/1.0E-24
      IF(I-2)26,27,28
   26 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),TMAX,
     1ACT1,ACT2
      GOTO23
   27 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),TMAX,ACT1,ACT2
      GOTO23
   28 WRITE(51,VAR)PHI(I),TMAX,ACT1,ACT2
      GOTO23
   25 ITMAX=8HNO MAX
      IACT1=ITMAX
      IACT2=ITMAX
      CALL NOMAX
      SIGMAA=SIGMAA/1.0E-24
      SIGMAB=SIGMAB/1.0E-24
      IF(I-2)326,327,328
  326 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),ITMAX,
     1IACT1,IACT2
      GO TO 23
  327 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),ITMAX,IACT1,IACT2
      GO TO 23
  328 WRITE(51,VAR)PHI(I),ITMAX,IACT1,IACT2
   23 CONTINUE
      GOTO2
    9 DO13I=1,NUMPHI
      SIGMAA=SIGMAA*1.0E-24
      SIGMAB=SIGMAB*1.0E-24
      IF(SIGMAB)97,11,97
   97 CALL YESMAX
      FACT1=0.69315/TA+PHI(I)*SIGMAA
      FACT2=PHI(I)*SIGMAB
      DENOM=FACT2-FACT1
      IF(DENOM)10,11,10
```

```
 10 IF(TMAXREAD)63,54,63
 54 TMAX=LOGF(FACT2/FACT1)/DENOM
    GOTO53
 63 TMAX=TMAXREAD
 53 ACT1=0.0
    ACT2=1.128E+13*ABUNA*EXPF(-FACT1*TMAX)/(TA*WTA)
    TMAX=TMAX/8.64E+4
 67 SIGMAA=SIGMAA/1.0E-24
    SIGMAB=SIGMAB/1.0E-24
    IF(I-2)14,15,16
 14 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),TMAX,
   1ACT1,ACT2
    GOTO13
 15 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),TMAX,ACT1,ACT2
    GOTO13
 16 WRITE(51,VAR)PHI(I),TMAX,ACT1,ACT2
    GOTO13
 11 ITMAX=8HNO MAX
    IACT1=ITMAX
    IACT2=ITMAX
    CALL NOMAX
    SIGMAA=SIGMAA/1.0E-24
    SIGMAB=SIGMAB/1.0E-24
    IF(I-2)314,315,316
314 WRITE(51,FMT)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,PHI(I),ITMAX,
   1IACT1,IACT2
    GO TO 13
315 WRITE(51,APE)ATOMB,SIGMAB,TBSTORE,UNITB,PHI(I),ITMAX,IACT1,IACT2
    GO TO 13
316 WRITE(51,VAR)PHI(I),ITMAX,IACT1,IACT2
 13 CONTINUE
    GOTO2
    END ISOTOPES
```

```
SUBROUTINE YESMAX
TYPE INTEGER FMT,APE,VAR
DIMENSIONFMT(10),APE(8),VAR(5)
COMMONFMT,VAR,APE
FMT(8)=6HE16.4,
FMT(9)=6HE14.4,
FMT(10)=6HE14.4)
VAR(3)=6HE16.4,
VAR(4)=6H2E14.4
VAR(5)=1H)
APE(6)=6HE16.4,
APE(7)=6HE14.4,
APE(8)=6HE14.4)
RETURN
END
```

```
SUBROUTINE NOMAX
TYPE INTEGER FMT,APE,VAR
DIMENSIONFMT(10),APE(8),VAR(5)
COMMONFMT,VAR,APE
FMT(8)=8H7X,A6,5X
FMT(9)=8H4X,A6,8X
FMT(10)=4H,A6)
VAR(3)=FMT(8)
VAR(4)=FMT(9)
VAR(5)=FMT(10)
APE(6)=FMT(8)
APE(7)=FMT(9)
APE(8)=FMT(10)
RETURN
END
```

```
      SUBROUTINE OPTION
      TYPE INTEGER FMT,APE,VAR
      DIMENSION FMT(10),APE(8),VAR(5)
      COMMONFMT,VAR,APE,ATOMA,SIGMAA,TA,UNITA,ABUNA,WTA,TMAXREAD,ATOMB,
     1SIGMAB,TB,UNITB,TASTORE,TBSTORE,OP
      IF(TB)1,2,1
    1 IF(TA)3,2,3
    3 FACTB=0.69315/TB
      FACTA=0.69315/TA
      DENOM=FACTB-FACTA
      IF(DENOM)5,2,5
    5 IF(TMAXREAD)7,6,7
    7 TMAX=TMAXREAD
      GOTO8
    6 TMAX=LOGF(TA/TB)/DENOM
    8 ACT1=7.81704E+12*ABUNA/(WTA*TB*TA)*(EXPF(-FACTA*TMAX)-EXPF(-FACTB*
     1TMAX))/DENOM
      ACT2=1.128E+13*ABUNA*EXPF(-FACTA*TMAX)/(TA*WTA)+ACT1
      TMAX=TMAX/8.64E+4
      WRITE(51,100)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA,TMAX,ACT1,
     1ACT2
  100 FORMAT(1H0,A8,2E14.5,A1,I3,F10.5,F9.3,7X,7H   ---   ,E18.4,2E14.4)
    4 WRITE(51,101)ATOMB,SIGMAB,TBSTORE,UNITB
  101 FORMAT(1H ,A8,2E14.5,A1)
      RETURN
    2 WRITE(51,102)ATOMA,SIGMAA,TASTORE,UNITA,OP,ABUNA,WTA
  102 FORMAT(1H0,A8,2E14.5,A1,I3,F10.5,F9.3,7X,7H   ---   ,2(9X,6HNO MAX),
     18X,6HNO MAX)
      GOTO4
      END
```

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