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OSCAR, A CODE FOR THE CALCULATION OF THE YIELD OF RADIOISOTOPES PRODUCED BY CHARGED-PARTICLE INDUCED NUCLEAR REACTIONS

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OSCAR, a Code for the Calculation of the Yield of Radioisotopes Produced by Charged-Particle Induced Nuclear Reactions

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A computer code OSCAR, operated on a main frame computer was developed for the calculation of the yield of radioisotopes produced by charged-particle induced nuclear reactions. The excitation functions required for calculating the yield were evaluated by means of an empirical rule which we developed on the basis of a systematics derived from a number of experimental data reported in the literature. The rule is valid for light ion ($Z \leqq 2$)-induced reactions followed by neutron emission processes. Other excitation functions are also obtainable from the data file in OSCAR. In addition, the code possesses functions useful for the calculation of the stopping power and range. The energy loss and the distribution of recoil products in stacked targets are also provided as options. The formalism, structure, and direction for the usage of the code are described together with the explanation of the functions of some routines.

Keywords: OSCAR Code, Yield of Radioisotopes, Nuclear Reaction

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荷電粒子反応により生成する放射性同位元素の生成量計算コード，OSCAR

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荷電粒子反応により生成する放射性同位元素の生成量を計算することを目的として，計算コードOSCARを大型計算機上で開発した。生成量の計算に必要な励起関数は，我々が開発した核反応断面積に関する経験則を使って計算する事ができる。ただし，この経験則は入射イオンが軽粒子（Z≦2）で，中性子放出反応に限って有効である。また，文献に記載された励起関数データを集めたデータファイルを利用する事もできる。このほかに加速器実験に際して役立つ付加的な機能として，阻止能と飛程，積層型ターゲット集合体中でのエネルギー損失およびその中での反跳核の分布が計算できる。計算方法，コードの構成と使用方法および有用なモジュールの仕様に付いて述べる。

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1. Introduction

We constructed a code, OSCAR, to calculate the yield of radioisotopes produced by charged-particle-induced reactions, throughly revising the previous code TYIELD[1] published in 1974. In order to evaluate the yield, numerical values of cross sections and stopping powers are required for an arbitrary combination of the projectile and target. In OSCAR, the excitation functions are calculated using an empirical rule which we developed on the basis of systematics derived from a number of experimental data reported in the literature. The rule, however, covers only light-ion induced reactions, with $Z \leqq 2$, followed by neutron emission processes since there are not a sufficient number of data available to extract any reliable systematics for other types of reaction. Instead, the excitation functions are either referred to in a computer file in which most of the numerical data reported in the literature from 1960 to 1987 were compiled or provided as input data by the use of an appropriate code like ALICE[2].

The calculation of the energy loss and range plays an important role as supplemental functions of OSCAR because they are indispensable information in beam experiments for the nuclear reaction study besides the technological applications of ion implantation and the use of ion beams in material science. For instance, one must know the magnitude of the energy loss in the target material to deduce the effective excitation energy for a relevant nuclear reaction. In-beam experiments using such as ISOL or helium-jet transport system require information on the rate of product nuclides recoiled out of the target which can be estimated using the recoil ranges. In practical work of radioisotope production using charged-particle accelerators, significantly thick targets are generally used in order to raise the yield of the product radioactivity. They are so thick as compared to the range of the projectile that they are considered to be of infinite thickness. Therefore, the total yield called "thick-target yield" should be deduced by means of the energy of incident particles at a given depth and the cross section value at the relevant energy.

Of universal formulas proposed for calculating the stopping power, we adopted the Ziegler's method[3] as the best which permits to judge the accuracy of calculation for various segments of possible combination of projectiles and targets. The stopping power can be calculated at energies above 0.1 keV for any projectile in solid targets. Functions necessary for the calculation of the stopping power and range were prepared, from which the magnitude of the energy loss in absorbing layers or the distribution of recoil products in a stacked target can be deduced.

Chapter 2 describes our empirical rule of the excitation function and the method of calculation of the stopping power, with which provided are the yield of a product nuclide, the energy loss in the absorbing layers and the distribution of the recoil products in the stacked target. Chapter 3 explains the structure of the code, the transfer of a source program to the load module and the structure of data files used in the code. Some routines in the code can also be used for other codes effectively and their structure and function are described in Chapter 4. Two types of execution of the code, BATCH processing and TSS processing, are available in OSCAR. Chapter 5 explains how to execute the code by these processes and shows samples of the input and output for BATCH processing. A user is recommended to read at least Chapter 5 and Tables 14 - 18 to use OSCAR.

2. Method of calculation

2.1 Yields of radioisotopes and excitation functions

The yield of a radioisotope Y, produced during irradiation of a target, is expressed as

$$Y = (N_A/M_2)N_P[1 - \exp(-\lambda t)] \int_{E_f}^{E_i} \{\sigma(E)/S(E)\}dE, \qquad (1)$$

where N_A is the Avogadro's number, M_2 the atomic weight of the target element, N_P the number of projectiles per unit time, λ the decay constant of the radioisotope, $\sigma(E)$ the cross section, and S(E) the stopping power of the target material at the ion energy E. E_i and E_f are the ion energies before and after passing through the target material. The stopping power is calculated using the semi-empirical formula reported by Ziegler et al.[3] for energies below 100 MeV/amu and the Bethe-Bloch equation[9] for energies above 100 MeV/amu which are described in detail in Appendix 1. Any theory to predict the formation cross sections for arbitrary radionuclides regardless of reaction mechanisms has not yet been totally established. In OSCAR, the following means of obtaining the excitation function needed for the calculation of the radioisotopic yield are provided: the excitation function is
(1) estimated with the empirical rule or
(2) obtained from the compiled file of experimental data.
If desired excitation functions can not be obtained by these means, a user have to prepare the input data set which would be obtained from existing computer codes or experimental data.

2.2 An empirical rule on the excitation function

A number of experimental data on cross sections for a variety of nuclear reactions have been reported. We compiled the cross section data for light-ion induced reactions followed by neutron emission processes, and established an empirical rule based on the systematics of the compiled excitation functions. The systematics has been derived based on qualitative arguments of the characteristics of the neutron decay of the excited nucleus left in the interaction between the projectile and target. This shall be described in detail in Appendix 3. As a result we obtained an equation to calculate the excitation function $\sigma(E)$ for the (q,xn)-type reaction, where q stands for the projectile:

$$\sigma(E) = \sigma_m (E_m/E)^c \frac{\exp(c) - 1}{[\exp(E_m/E)]^c - 1}, \tag{2}$$

where σ_m is the cross section (mb) at the laboratory energy E_m (MeV) of the peak of the excitation function. c is the parameter dependent of the reaction system determined by fitting Eq.(2) to the compiled data:

$$\begin{cases} c = C_L & \text{for } E \leqq E_m, \quad (3) \\ c = C_L + 10 & \text{for } E > E_m, \quad (4) \end{cases}$$

with

$$\begin{cases} C_L = A_c/10 + 10(x - 1) & \text{for the (p,xn) reactions,} \\ C_L = A_c/10 + S[10(x - 2)] & \text{for the (d,xn),(}^3\text{He,xn) and } (\alpha\text{,xn) reactions,} \end{cases}$$

where A_c is the mass number of compound nuclei. S(x) is a step function defined as

$$\begin{cases} S(x) = 0 & \text{for } x < 0, \\ S(x) = x & \text{for } x \geqq 0. \end{cases}$$

E_m is given by

$$E_m = E_{max}(A_1 + A_2)/A_2 \tag{5}$$

with

$$E_{max} = E_M' + 2\sum_{i=1}^{x} T_i, \tag{6}$$

$$E_M' = S\{\min[B_n(x+1),\ B_p(x+1) + 0.2E_c^{(p)}] - Q(q,xn)\} + 0.4S[E_c^{(q)} + Q(q,xn) - Z_1 - 4.5], \qquad (7)$$

and

$$T_i = \{\ [E_M' + Q(q,in)]/a_i\ \}^{1/2},$$

where E_{max} designates the peak position of the excitation function in the center-of-mass (CM) system, A_1 and A_2 denote the mass numbers of the projectile and the target nuclei. Z_1 is the nuclear charge of the projectile and B_n and B_p give the binding energies of neutron and proton, respectively, in the residual nuclei. $E_c^{(q)}$ is the Coulomb barrier for the projectile q in the target nuclei and $E_c^{(p)}$ the Coulomb barrier for proton in the residual nuclei. Q(q,xn) represents the Q_{gg} values of the (q,xn)-type reaction. The level density parameter a_i of the residual nuclei is estimated from a semi-empirical formula[4] based on the shell model.
σ_m is given by

$$\sigma_m = \sigma_g P_n \exp(-f_{Ecm} - f_{Ec} - f_{dN}), \qquad (8)$$

with

$$\sigma_g = 10\pi\ (r_0A_2^{1/3} + \lambda\ )^2, \qquad (9)$$

where σ_g is the geometrical cross section (mb), r_0 the nuclear radius parameter (taken to be 1.25fm) and λ the reduced de Broglie wave length (fm). The neutron emission probability P_n against the competing fission is represented by the relation:

$$P_n = \prod_{i=1}^{x} P_{n,i}, \qquad (10)$$

$$P_{n,i} = 1/[1 + \Gamma_{f,i}/\Gamma_{n,i}], \qquad (11)$$

with

$$\Gamma_{f,i}/\ \Gamma_{n,i} = 0 \qquad \text{for } Z_c \leqq 90, \qquad (12)$$

$$\Gamma_{f,i}/\ \Gamma_{n,i} = \exp[a(Z_c(i)^2/A_c(i) - b)] \qquad \text{for } Z_c > 90,$$

where

$$a = 1.53,$$

$$b = \begin{cases} 36.0, & \text{for } Z_c \leqq 94, \\ 36.0 + 0.975N - 0.075N^2, & \text{for } Z_c > 94, \end{cases}$$

and

$$N = (Z_c(1) - 93)/2,$$

$\Gamma_{f,i}$ and $\Gamma_{n,i}$ are the level widths of fission and neutron emission channels respectively.
The attenuation factors f_{Ecm}, f_{Ec} and f_{dN} in the exponent of Eq.(8) are

$$f_{Ecm} = S[\Delta E_{cm} - 6)]/8, \qquad (13)$$

with

$$\Delta E_{cm} = E_{cm} - E_0,$$
$$E_{cm} = E_{max} - S[-Q(q,xn)],$$
$$E_0 = S\{E_{cm} - S[-Q(q,n)]\} + 7.0,$$

$$f_{Ec} = 0.4S[E_c^{(q)} + Q(q,xn) - Z_1 - 4.5], \qquad (14)$$

and

$$f_{dN} = 0.116S[\Delta n - 3.9] + \ln 2, \qquad (15)$$

with

$$\Delta n = \{M(Z_c,A_3) - M(Z_c,A_0)\}S[A_0 - A_3] - \{M(Z_c,A_c) - M(Z_c,A_0)\}S[A_0 - A_c].$$

Here, M(Z,A) represents the mass excess (MeV) of the nuclide with nuclear charge Z and mass number A. A_3 is the mass number of the residual nuclei and A_0 the mass number of the nuclide with a minimum value of mass excess among isotopes with atomic number Z_c. The accuracy of the calculated σ_m was within a factor of 2 and that of the calculated E_m was ± 2 MeV. The comparison between calculated and experimental excitation functions is shown in Fig. 9 for ^{209}Bi(p,xn) reactions and in Fig.10 for the ^{197}Au(α,xn) reactions.

2.3 The energy loss in stacked targets

If the thickness T of a target material is smaller than the projected range R at the initial ion energy E_0, the energy loss in the target is expressed as

$$\Delta E = E_0 - E_{R-T}, \quad (16)$$

where E_{R-T} is the ion energy corresponding to a projected range R-T estimated from the Biersack's formula[3,5] which is described in detail in Appendix 2. The incident energy on the i-th material in stacked targets is given by

$$E_i = E_{i-1} - \Delta E_{i-1}, \quad (17)$$

where E_{i-1} and ΔE_{i-1} are the incident energies of ions entered in the (i-1)th material and the energy loss in the (i-1)th material, respectively.

2.4 Distribution of recoil products in stacked targets

A stacked target used in radiochemical works often consists of thin foils containing target nuclei and some metal foils for catching recoil products originated by the nuclear reactions. (If the recoil nucleus is a fission product with large kinetic energy, the catcher foils are to be set also in front of the target foil.) The thickness of the individual foil must be less than the projected range of the recoil product in the foil except for the last catcher foil. It is important that the catcher foil does not contain any nuclides which may interfere the relevant product. When ions with the laboratory energy E_1 enter the target foil and nuclear reactions take place, the nucleus of interest scatters with the laboratory energy E_3 and pass through the catcher foils. In OSCAR, the kinetic energy of recoil products originated by three types of nuclear reactions can be estimated as described below, the angular distribution of recoil products in the CM system being assumed to be isotropic.

(1) Evaporation products decayed from compound nuclei

Recoil energy E_3' in the CM system is derived from the non-relativistic two body kinematics:

$$E_3' = (E_1' + Q)\ A_4/(A_3 + A_4), \tag{18}$$

with

$$E_1' = E_1\ A_2/(A_1 + A_2),$$
$$A_4 = A_1 + A_2 - A_3,$$

where A_3 is the mass number of the residual nucleus, Q the Q-value of the reaction and E_1' the incident energy in the CM system.

(2) Fission products

Total kinetic energy E_k (MeV) of the fission products from the symmetric fission process can be estimated from the Viola's systematics[6]:

$$E_k = 0.1071\ Z_c^2/A_c^{1/3} + 22.3. \tag{19}$$

$E_3'(\theta)$ is calculated from Eq.(18) with $Q = E_k - E_1'$.

(3) Products from asymmetric fission and damped collision processes[22]

Total kinetic energy E_k (MeV) of products from the strongly damped collision can be estimated based on the Viola's systematics:

$$E_k = 4(0.1071 Z_c^2/A_c^{1/3} + 22.3)\ Z_1 Z_2/Z_c^2 \tag{20}$$

$E_3'(\theta)$ is calculated from Eq.(18) with $Q = E_k - E_1'$.
The scattering angle θ' in the CM system to be calculated, is determined by dividing π radian in equal parts by a dividing

number N_g. (The default value of N_g is 100.) The kinetic energy $E_3(\theta)$ in the laboratory system is obtained from E_3' as follows;

$$E_3(\theta') = E_3'(1 + K^2 + 2K\cos\theta'), \tag{21}$$

$$K = \{ \frac{A_1A_3}{A_2A_4} \frac{E_1'}{(E_1' + Q)} \}^{1/2}, \tag{22}$$

and θ' is converted to the scattering angle in the laboratory system:

$$\theta = \tan^{-1}\{\sin\theta'/(\cos\theta' + K)\}. \tag{23}$$

Next, the energy loss ΔE in the target is estimated for the recoil nucleus as ejected in the direction θ with energy $E_3(\theta)$. If the residual energy $E_3-\Delta E$ is larger than zero, this energy is taken to be the incident energy for the next catcher foil to repeat the calculation of ΔE. Such a calculation is continued as long as catcher foils exist. Finally, the distribution D_s is determined by counting the number of the events of stopping of the recoil products in every foil:

$$D_s = \frac{\sum_{j=1}^{N_s} \sin\theta_j'(1 + a\cos^2\theta_j')}{\sum_{I=1}^{N_g} \sin\theta_I'(1 + a\cos^2\theta_I')}, \tag{24}$$

where

$$\theta_i' = [\sum_{i=1}^{I} \frac{\pi}{Ng}] + \frac{\pi}{2Ng}, \tag{25}$$

Here, a is the anisotropy factor for angular distribution of fission products and becomes zero for the isotropic distribution. In the case where the target thickness can not be neglected compared to the projected range of the recoil nuclei in the target, the target thickness is partitioned into several parts. The distributions are calculated for individual parts of the target in which the energy loss of recoil products can be neglected, and the final results are given by adding all of the individual distributions. The excitation function must be taken into consideration at calculation of the distribution of recoil products when the energy loss of the ions in the target foil is so large that the cross section is hardly considered to be constant throughout the target.

3. Contents of OSCAR

OSCAR was developed using a main frame computer FACOM M380R. The programing language is FACOM OS IV/F4 MSP FORTRAN77 (when OSCAR is to be used in other FORTRAN77 systems, the FORTRAN77 statement including "DO WHILE" or "DO UNTIL" should be translated into appropriate one). Configuration of the code is shown in Fig.1. Two types of load modules for input/output (I/O) are provided. One is OSCAR3B.LOAD for BATCH processing which has a user's source file as a standard input device and a printer as a standard output device. The other is OSCAR3T.LOAD for TSS processing which has a terminal as a standard I/O device. These load modules are linked to a private library, OSCAR3L.LOAD that contains subprograms common in OSCAR. Also, there are data files for I/O, OSIO.DATA and for data base: SIGMA.DATA and MASWPS.DATA.

(1) Private library: OSCAR3L.LOAD

This load module contains subprograms common in OSCAR. Table 1 briefly shows the functions of the subprograms. The original source file of the load module is OSCAR3L.FORT77 that requires the storage capacity of about 350 k bytes. An example of TSS command procedure for preparing the load module as a private library from the source file is

```
FORT77 OSCAR3L ELM(*) NAME
LINK OSCAR3L.OBJ LET NCAL
```

(2) Load module for I/O in TSS processing: OSCAR3T.LOAD

Execution of I/O in TSS processing is done by means of this module that has the functions of indicating menus and prompts for arrangement of input data on the terminal display, reading of the input data from the terminal keyboard, calculation with the input data, and indication of the calculated results on the display. The original source file is OSCAR3T.FORT77 that requires storage capacity of about 100 k bytes. An example of TSS command procedure for preparation of the load module from the source file and private library is

```
FORT77 OSCAR3T
LKED77 LM(OSCAR3T.LOAD) PRVLIB('OSCAR3L.LOAD')
```

(3) Load module for I/O in BATCH processing: OSCAR3B.LOAD

This module used for executing I/O in BATCH processing has functions of the reading of input data, calculation with the input data, and print out of the calculated results. The original source file is OSCAR3B.FORT77 that requires the storage capacity of about 80 k bytes. An example of TSS command procedure for preparing the load module from the source file is

```
FORT77 OSCAR3B
LKED77 LM(OSCAR3B.LOAD) PRVLIB('OSCAR3L.LOAD')
```

(4) Data file of excitation function: SIGMA.DATA

This is an unformatted direct data set with record length of 2 k bytes. The record number in the data file correspond to the orders of entering of input data. The file contains compiled numerical data appeared in the literature dating from 1960 to 1987. The number of data is 1526 at the end of 1987. The formats and meanings of data elements are indicated in Table 2.

(5) Data file of nuclear mass excess: MASWPS.DATA

This is a formatted sequential data set that contains the nuclear mass excess data reported by Wapstra et al.[7] Table 3 shows the formats and meanings of data elements.

(6) Data file for I/O: OSIO.DATA

This is a partitioned data set accessible from the editor on the terminal. There exist the members of I/O data to be accessed from OSCAR3T.LOAD and/or OSCAR3B.LOAD. Four members: IPT1, IPT2, IPT3 and IPT4 are input data sets for calculating the yield of radioisotopes, energy loss in stacked targets, stopping power and the range and distribution of recoil products in stacked targets, respectively. These input data sets can be used in BATCH processing by adding appropriate job control statements because the data sets have the same format as one of the input data in BATCH processing. The other two members OPTT and OPTB are output data sets for TSS processing and BATCH processing, respectively.

(7) Data file of input data set in BATCH processing

A user should prepare the data file that consists of input data set and job control statements.

4. Specification of useful subprograms in the library

The subprograms in OSCAR3L.LOAD can be called from other programs and effectively used. The structure and usage of useful subprograms is explained below.

4.1 Calculation of radioisotope yield: SUBROUTINE YIELDZ

This subroutine is used for the calculation of the yield of radioisotopes produced by charged-particle induced reactions. The subroutine statement is

```
SUBROUTINE YIELDZ( IW,E,IMAX,MP,NP,AMOL,TGD,ITG,EEX,CRS,NEX,
ABDC,YLS ).
```

The data types and meanings of the arguments are indicated in Table 4. Other input data are to be in the following common block to calculate the yield of radioisotopes:

```
COMMON /RGZCO/IER,IZ1,IA1,NKD,NEL(20),IZ2(20),A2(20),
POTC(20),DSTC(20)
```

The data types and meanings of the variables are given in Table 5. Fig.2 shows the tree structure of subprograms called from the subroutine. The function of all of the called subprograms are explained in Table 1.

4.2 Calculation of excitation function: SUBROUTINE SGCAL1

This subroutine is used for the estimation of the excitation function using the empirical formula. The subroutine statement is

```
SUBROUTINE SGCAL1(IW,Z1,A1,Z2,A2,N4,Z4,A4,EMAXI,SMAXI,NENG,
ENG,SIG ).
```

Table 6 indicates the data types and meanings of the arguments. The tree structure of the subprograms called from the subroutine is shown in Fig.3.

4.3 Calculation of the energy loss in stacked targets: FUNCTION DELENZ

This double precision function is used for the calculation of the energy loss in stacked targets. The function statement is

```
DOUBLE PRECISION FUNCTION DELENZ( E1,TD ).
```

The data types and meanings of the arguments are shown in Table 7. The variables in the common block RGZCO are needed to calculate the energy loss (cf. section 4.1). Fig.4 indicates the tree structure of the subprograms called from the function.

4.4 Calculation of stopping powers: SUBROUTINE SPWZCO

This subroutine is used for the calculation of the stopping power of projectiles in target materials. The subroutine statement is

```
SUBROUTINE SPWZCO(E,IZ1,IA1,IZ2,A2,NEL,NKD,POTC,DSTC,IER,
IUNIT,ST,SE,SN ).
```

The data types and meanings of the arguments are shown in Table 8. The tree structure of the subprograms called from the subroutine is indicated in Fig.5.

4.5 Calculation of projected ranges: FUNCTION RGPZCO

This double precision function is used for calculation of the projected range of projectiles in target materials. The function statement is

```
DOUBLE PRECISION FUNCTION RGPZCO( ENG ).
```

The types and meanings of the arguments are shown in Table 9. The variables in common block RGZCO are needed to calculate the projected range (cf. section 4.1). Fig.6 indicates the tree structure of the subprograms called from the function.

4.6 Calculation of distribution of recoil products: SUBROUTINE RCLDSZ

This subroutine is used for the calculation of the distribution of recoil products in stacked targets. The subroutine statement is

```
SUBROUTINE RCLDSZ(IW,IZ1,IA1,IZ2,IA2,IZ3,IA3,N4,IZ4,IA4,
JZ2,AA2,IRCT,Q,E1L,NFL,NTGT,ITG,TGD,NKD,NEL,NANG,ANS1,
ANS2,NEX,EEX,CRS,NP,MP,IPRT,PCTF,PCTB,EIN,TGS ).
```

Table 10 lists the data types and meanings of the arguments. The tree structure of the subprograms called from the subroutine is shown in Fig.7.

4.7 Retrieving of excitation function data: SUBROUTINE DATSIG

This subroutine is used for the retrieval of the desired excitation function from the data base SIGMA.DATA. The subroutine statement is

```
SUBROUTINE DATSIG( IW ).
```

Table 11 shows the data type and meaning of the arguments. The tree structure of the subprograms called from the subroutine is shown in Fig.8.

4.8 Data of elements: SUBROUTINE ELMDA3

This subroutine is used for passing the data of elements in the following common blocks to call subprograms and has no argument:

```
COMMON /ELM/ ELN(0:110)
COMMON /ATMZ/ ATW(92),DSTY(92),FRMV(92),FSCR(92),COFP(92,8)
```

```
COMMON /STHM/ X0(110),X1(110),AA(110),AM(110),D0(110),
POT(110)
```

The first subscript of the array corresponds to the atomic number of an element. The data types and meanings of the variables are shown in Table 12.

5. Direction for using OSCAR

Two input modes were prepared in OSCAR. One is for the BATCH processing which is somewhat troublesome for use because the input formats are strictly defined but is convenient when numerous input data are to be prepared. The other is for TSS processing without any format control for the input.

5.1 Batch processing

This input data set consists of the job control statements and input data. OSCAR with the input data set is executed by means of the command "SUBMIT". The typical job control statements are shown in Table 13 and the input formats are shown in Table 14. Tables 15 - 18 indicate samples of I/O for individual calculations. The test data for confirming the execution of the code were saved in OSIO.DATA(TESTDT) for the input and OSIO.DATA(TESTRS) for the output.

5.2 TSS processing

Execution in the TSS processing requires command procedures to run OSCAR3T.LOAD. An example of the command procedure is shown in Table 19. The code begins to run by a command "OT" that is a member name in TSSMAC.CLIST. The following menu and prompt are indicated on the terminal display:

```
 ------------------------------------------------------------
 !  PLEASE, CHOOSE THE NUMBER OF FUNCTION TO BE EXECUTED.      !
 ! +------------------------------------------------------+   !
 !    1. REACTION PRODUCT YIELD                                 !
 !    2. ENERGY LOSS IN MEDIUM                                  !
 !    3. STOPPING POWER AND RANGE                               !
 !    4. DISTRIBUTION OF RECOIL PRODUCTS IN STACKED-TARGET      !
 !    5. SHOW EXCITATION FUNCTION DATA IN DATA BASE             !
 ! +------------------------------------------------------+   !
 ! Q: NUMBER(END -> 0) ===>                                    !
 ------------------------------------------------------------
```

When the number of desired menu is entered following the prompt that is indicated at the bottom of the screen, the next menu for the desired calculation is indicated. Thus all the input data required for the calculation can be entered following the direction of menus and prompts on the screen. The meaning and default values of individual input data can be referred to Table 14. It is important for easy entering that the input data with a default value should not be entered if the default value is reasonable for the calculation. When the number 90 is entered for execution after complete arrangement of the input data, the calculation starts and the calculated results are shown on the display. If a user wish to save the calculated results in the data file OSIO.DATA(OPTT), one can execute the action by means of specifying "FILE" in the prompt "INSTRUMENT FOR PRINT". Also, the save and load of the input data set into OSIO.DATA(IPT1) - (IPT4) are executed by means of specifying the numbers 92 and 91, respectively, as shown in the prompt. Such a saved input data set is used for BATCH processing if appropriate job control statements are added.

6. Discussion

Accuracy of calculation of the yield of radioisotopes is strongly dependent on that of the excitation function. In OSCAR, our empirical rule was used to evaluate the excitation function which has not yet been established. The effectiveness of the rule is limited to light-ion induced reactions followed by neutron emission. The rule is, however, simple with sufficient accuracy and quite practical because

1) more than 80 % of radioisotopes useful for practical application have been produced utilizing light-ion nuclear reactions with particle accerelators. Furthermore, they are mostly produced with the highest yield when the (q,xn) type of reaction is available. The same situation would be predicted for radioisotopes which have been found to be potentially useful in the future.

2) The CPU time necessary for calculation of an excitation function using the empirical rule is less than 1 s.

The calculation based on the empirical rule provides an accuracy of a factor 2 for the maximum cross section and ± 2 MeV for the projectile energy at the maximum cross section. Currently available computer codes used for the calculation of the excitation function are not necessarily useful or practical from the quantitative point of view. The main reason is that accuracy of calculation with the model calculations is more or less dependent on adjustable parameters which are not uniquely determined for a given combination of target and projectile. For example, when radioisotopes are produced by deuteron- or ^{3}He-induced reactions followed by neutron emission, the compound nucleus formation processes and direct reactions are involved as well. In this case, the yield of radioisotopes can not be evaluated precisely based on the statistical model only. Thus all reaction channels must be calculated in order to evaluate the yield of radioisotopes precisely. Any nuclear theories or models on reaction mechanisms except for the compound nucleus reaction have not yet been definitely established until now. Since the empirical rule covers both of the reaction channels and has no adjustable parameters, this rule is of greater advantage than any theoretical calculations, although the validity of the rule is restricted to the neutron emission process. In any case universal methods for evaluating the yield of radio- isotopes will be established in the near future since efforts are continued to develop the nuclear reaction theory and computation technique.

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Table 1 Module types and functions of subprograms in the library OSCAR3L.LOAD
Module type S represents SUBROUTINE, SF single precision FUNCTION and F double precision FUNCTION

Module Name	Module Type	Function
		--- Modules relevant to calculation of the yield of radioisotopes ---
GRAPH	S	Draws one set or two sets of two-dimensional data graphically, using character type
LSTSQR	S	Fits two-dimensional data by polynomial
SIGTOZ	F	Integrates the ratio of cross section to stopping power for projectile energy
SMOOTH	S	Performs smoothing of two-dimensional data
YIELDZ	S	Calculates the yield of radioisotopes
CLMENG	F	Calculates the Coulomb energy of two spheres in contact
ENGMAX	SF	Calculates the projectile energy for the maximum cross section in a given reaction system using the empirical rule
LEVEL	S	Calculates the level density parameter of residual nuclei using Baba's semi-empirical formula[4)]
SGCAL1	S	Calculates the excitation function of a given reaction system using the empirical rule
SIGFRM	S	Calculates the form of the excitation function of a given reaction system using the empirical rule
SIGMAX	SF	Calculates the maximum cross section of a given reaction system using the empirical rule

Table 1 continued

		--- Modules relevant to calculation of the stopping powers ---
BETA2	F	Calculates the square of the ratio of par ticle velocity to light velocity
MASRED	S	Reads all the nuclear mass data from MASWPS.DATA and enters them in arrays
MASSEL	F	Obtains the nuclear mass with a given atomic number and mass number from the array
DSTEFC	F	Calculates the density effect for stopping powers
SPWBET	F	Calculates the electronic stopping power at energies above 100 MeV/amu using the Bethe-Bloch equations[9]
SPWZCO	S	Calculates the nuclear, electronic and total stopping power in the solid material composed of mono-atoms or different atomic species
SPWZEL	S	Calculates the nuclear, electronic and total stopping power in the solid material composed of mono-atoms
SPWZHE	F	Calculates the electronic stopping power for He ions at energies below 100 MeV/amu using the Ziegler's formula[3]
SPWZHI	F	Calculates the electronic stopping power for heavy ions (Z > 2) at energies below 100 MeV/amu using the Ziegler's formula
SPWZNU	F	Calculates the nuclear stopping power using the Ziegler's formula
SPWZPR	S	Calculates the electronic stopping power for protons at energies below 100 MeV/amu using the Ziegler's formula

Table 1 continued

		--- Modules relevant to calculation of the projected ranges ---
ITGGAU	F	Evaluates the numerical solution of one-dimensional-differential equation by means of the Gauss-Legendre method
RGPZCO	F	Calculates the projected range in the solid material composed of mono-atoms or different atomic species
		--- Modules relevant to calculation of the energy loss in the stacked target ---
DELENZ	F	Calculates the energy loss in the stacked target
VARCVZ	S	Converts two-dimensional array to one-dimensional array for the variables of target materials
		--- Modules relevant to calculation of the distribution of recoil products ---
ANGCVT	F	Transforms the scattering angle of products in the laboratory system to that in the CM system or vice versa, assuming the two-body kinematics
ENGCVT	F	Transforms the kinetic energy of products in the laboratory system to that in the CM system or vice versa, assuming the two-body kinematics
EVPKEN	F	Calculates the kinetic energy of evaporation residues assuming full momentum transfer

Table 1 continued

FSNKEN	F	Calculates the total kinetic energy for symmetric or asymmetric fissions
QGGVAL	F	Calculates the ground-state Q-value for a given nuclear reaction using Wapstra's mass data[7)]
RATVC3	F	Calculates the ratio of product velocity to center-of-mass velocity
RCLDSZ	S	Calculates the distribution of recoil products in the stacked target
		--- Modules relevant to retrieving of the excitation function data ---
DATSIG	S	Shows the excitation function data for a given nuclear reaction retrieved from the data file SIGMA.DATA
SHOWME	S	Shows the excitation function data of a given record number in the data file SIGMA.DATA
SRTENG	S	Sorts the projectile energies of a given excitation function in ascending order
SRTRCT	S	Retrieves the excitation function data for a given nuclear reaction from the data file SIGMA.DATA
		--- Others ---
ELMDA3	S	Is referred the data relevant to elements from other subprograms
RCTEQU	S	Prints reaction formulas for a given reaction system

Table 2 Format of the excitation function data in SIGMA.DATA

Item of Data	Data Type	Remark
Literature	CHARACTER *80	Journal, Volume, Page, and Published year
Authors	CHARACTER *80	
Specification of reaction mechanism	CHARACTER *2	'TR' : Reaction cross section, 'SP' : Spallation cross section, 'FU' : Fusion cross section, 'FS' : Fission cross section, ' ' : Others
The energy level of product nuclei	CHARACTER *1	'M' : Meta-stable, 'G' : Ground-state, ' ' : Others
The unit of errors in projectile energies	CHARACTER *3	'MEV' or ' ': Units in MeV, '% ': Units in %
The unit of errors in cross sections	CHARACTER *2	'MB' or ' ' : Units in mb, '% ' : Units in %
Projectile atomic number	REAL*4	
Projectile mass number	REAL*4	
Target atomic number	REAL*4	

Table 2 continued

Target mass number	REAL*4	
Product atomic number	REAL*4	
Product mass number	REAL*4	
(1) The number of ejectiles	INTEGER	
Ejectile atomic number	REAL*4	
Ejectile mass number	REAL*4	
(2) The number of ejectiles	INTEGER	
Ejectile atomic number	REAL*4	
Ejectile mass number	REAL*4	
(3) The number of ejectiles	INTEGER	
Ejectile atomic number	REAL*4	
Ejectile mass number	REAL*4	
The number of cross sections	INTEGER	
(1)		Energies, cross sections and their errors are aligned by the number specified above
Projectile energy(MeV)	REAL*8	
Error in energy	REAL*8	
Cross section(mb)	REAL*8	
Error in cross section	REAL*8	
(2)		
Projectile energy(MeV)	REAL*8	
Error in energy	REAL*8	
Cross section(mb)	REAL*8	
Error in cross section	REAL*8	

Table 3 Format of the nuclear mass data in MASWPS.DATA.
11 lines (character type) from the top of the file are the explanation for the mass data followed by the following format:

Item of data	Data type
Atomic number	I6
Mass number	I6
Mass excess (MeV)	3X,F10.6
Error in mass excess (keV)	3X,F10.6

Table 4 Arguments of SUBROUTINE YIELDZ

Variable Name	Format (DIMENSION)	Remark
		--- Input Data ---
IW	INTEGER	The unit specifier for printing of results of smoothing of the excitation function
E(I)	REAL*8 (IMAX)	Projectile energies (MeV) [I = 1,IMAX]
IMAX	INTEGER	The number of energies to be calculated
MP*	INTEGER	The degrees of polynomial used in smoothing of the excitation function data (The default value is 3)
NP*	INTEGER	The number of smoothing points (The default value is 5)
AMOL	REAL*8	The atomic weight for the target composed of mono-atoms, or molecular weight for that composed of different atomic species
TGD	REAL*8	The thickness of target material (mg/cm^2), TGD = 0 for calculation of thick-target yields, = -TGD for calculation of thin-target yields**
ITG	INTEGER	ITG is always 0
EEX(J)	REAL*8 (NEX)	Projectile energies (MeV) in the excitation function data [J = 1,NEX]

Table 4 continued

CRS(J)	REAL*8 (NEX)	Cross sections (mb) in the excitation function data [J = 1,NEX]
NEX	INTEGER	The number of cross sections in the excitation function data
ABDC	REAL*8	The abundance of the target nuclide
		--- Output Data ---
YLS(I)	REAL*8 (IMAX)	The yield (μCi/μA) of a radio-isotope at infinite irradiation time

* To obtain the smoothing cross section at a given projectile energy, the excitation function data are fitted by MP-degree polynomial for NP data centered in the energy.

** It is assumed that the yield is proportional to the thickness of the target material.

Table 5 List of COMMON /RGZCO/

Variable Name	Format (DIMENSION)	Remark
IER	INTEGER	This value is always 0
IZ1	INTEGER	Projectile atomic number
IA1	INTEGER	Projectile mass number
NKD	INTEGER	The number of kinds of elements in the target material
NEL(I)	INTEGER (20)	When the target material is composed of mono-atoms, this value is 1. When the material is composed of different atomic species, this value is the composition ratio of i-th element in the compound [I=1,NKD]
IZ2(I)	INTEGER (20)	The atomic number of I-th element [I = 1,NKD]
A2(I)*	REAL*8 (20)	The atomic weight of I-th element [I = 1,NKD]
POTC(I)*	REAL*8 (20)	The mean excitation potential (eV) of orbital-electrons in I-th element [I = 1,NKD]
DSTC(I)*	REAL*8 (20)	The solid density (g/cm^3) of I-th element [I = 1,NKD]

* This value is obtained from SUBROUTINE ELMDA3.
(cf. Section 4.8)

Table 6 Arguments of SUBROUTINE SGCAL1

Variable Name	Format (DIMENSION)	Remark
		--- Input Data ---
IW	INTEGER	The unit specifier for printing of intermediate results of calculation
IPRT	INTEGER	The control index for printing of intermediate results of calculation, IPRT = 0 for no printing, = 1 for printing
Z1	REAL*4	Projectile atomic number
A1	REAL*4	Projectile mass number
Z2	REAL*4	Target atomic number
A2*	REAL*4	Target mass number
N4(I)	INTEGER (3)	N4(1) is the number of neutrons emitted. The other are always 0
Z4(I)	REAL*4 (3)	all the value is always 0
A4(I)	REAL*4 (3)	A4(1) is 1. The other are always 0
		--- Output Data ---
EMAXI	REAL*4	The energy (MeV) at the maximum cross section.
SMAXI	REAL*4	The maximum cross section (mb)
NENG	INTEGER	The number of cross sections (mb) in the excitation function
ENG(J)	REAL*4 (300)	The energies (MeV) in the excitation function [J = 1,NENG]
SIG(J)	REAL*4 (300)	The cross sections (mb) in the excitation function [J = 1,NENG]

* This value is obtained from SUBROUTINE ELMDA3.
(cf. Section 4.8)

Table 7 Arguments of DOUBLE PRECISION FUNCTION DELENZ

Variable Name	Format (DIMENSION)	Remark
		--- Input Data ---
E1	REAL*8	Projectile energy (MeV)
TD	REAL*8	The thickness (mg/cm^2) of the target material
		--- Output Data ---
DELENZ	REAL*8	The energy loss (MeV) in the target material

Table 8 Arguments of SUBROUTINE SPWZCO

Variable Name	Format (DIMENSION)	Remark
		--- Input Data ---
E	REAL*8	Projectile energy (MeV)
IZ1	INTEGER	Projectile atomic number
IA1	INTEGER	Projectile mass number
IZ2(I)*	INTEGER (20)	The atomic number of I-th element in the target material [I = 1,NKD]
A2(I)*	REAL*8 (20)	The atomic weight of I-th element in the target material [I = 1,NKD]
NEL(I)	INTEGER (20)	When the target material is composed of mono-atoms, this value is 1. When the material is composed of different atomic species, this value is the composition rate of I-th element in the compound [I = 1,NKD]
NKD	INTEGER	The number of kinds of elements in the target material
POTC(I)*	REAL*8 (20)	The mean excitation potential (eV) of orbital electrons in I-th element. [I = 1,NKD]
DSTC(I)*	REAL*8 (20)	The solid density (g/cm^3) of I-th element [I = 1,NKD]
IER	INTEGER	This value is always 0
IUNIT	INTEGER	The control index for the unit of stopping powers to be calculated, IUNIT = 0: MeV/(mg/cm^2), = 1: eV/(10^{15}atoms/cm^2)
		--- Output Data ---
ST	REAL*8	Total stopping power
SE	REAL*8	Electronic stopping power
SN	REAL*8	Nuclear stopping power

* This value is obtained from SUBROUTINE ELMDA3.
(cf. Section 4.8)

Table 9 Arguments of DOUBLE PRECISION FUNCTION RGPZCO

Variable Name	Format	Remark
		--- Input Data ---
ENG	REAL*8	Projectile energy (MeV)
		--- Output Data ---
RGPZCO	REAL*8	Projected range (mg/cm^2)

Table 10 Arguments of SUBROUTINE RCLDSZ

Variable Name	Format (DIMENSION)	Remark
		--- Input Data ---
IW	INTEGER	The unit specifier for printing of intermediate results of calculation
IZ1	INTEGER	Projectile atomic number
IA1	INTEGER	Projectile mass number
IZ2	INTEGER	Target atomic number
IA2	INTEGER	Target mass number
IZ3	INTEGER	Product atomic number
IA3	INTEGER	Product mass number
N4(I)*	INTEGER (3)	The number of ejectiles [I = 1,3]
IZ4(I)	INTEGER (3)	Ejectile atomic number [I = 1,3]
IA4(I)	INTEGER (3)	Ejectile mass number [I = 1,3]
JZ2(J,K)	INTEGER (20,20)	The atomic number of K-th element in J-th material which constitutes the stacked target [J = 1,NFL], [K = 1,NKD(J)]
AA2(J,K)	REAL*8** (20,20)	The atomic weight of K-th element in J-th material which constitutes the stacked target [J = 1,NFL], [K = 1,NKD(J)]
IRCT	INTEGER	The control index for nuclear reaction mechanism, IRCT = 0: Evaporation process from compound nuclei assuming full momentum transfer

Table 10 continued

		= 1: Symmetric fission process,
		= 2: Asymmetric fission
Q	REAL*8	Reaction Q-value (MeV). If Q is 0, it is calculated as Q_{gg}-value using Wapstra's mass data (IRCT = 0) or is calculated from the kinetic energy of fission products (IRCT = 1,2)
E1L	REAL*8	Projectile energy (MeV)
NFL	INTEGER	The number of constituent materials of the stacked target
NTGT	INTEGER	The number of dividing of the material which contains target nuclides. The default value is 1 (cf. Section 2.4)
ITG	INTEGER	The order of the material which contains target nuclides in the stacked target (The material faced on incident beams is specified as 1)
TGD(J)	REAL*8 (20)	The thickness of J-th material (mg/cm^2) [J = 1,NFL]
NKD(J)	REAL*8 (20)	The number of kinds of constituent elements of J-th material [J = 1,NFL]
NEL(J,K)	INTEGER (20,20)	When J-th material is composed of mono-atoms, this value is 1. When the material is composed of different atomic species, this value is the composition ratio of K-th element in the compound [J = 1,NFL], [K = 1,NKD(J)]

Table 10 continued

NANG	INTEGER	The number of dividing of π radian in CM system (cf. Section 2.4)
ANS1	REAL*8	The anisotropy coefficient in angular distribution of fission products
ANS2	REAL*8	This value is always 0
NEX	INTEGER	The number of cross sections in the excitation function
EEX(L)	REAL*8 (NEX)	Projectile energies (MeV) in the excitation function [L = 1,NEX]
CRS(L)	REAL*8 (NEX)	Cross sections (mb) in the excita-ation function [L = 1,NEX]
NP***	INTEGER	The number of smoothing points (The default value is 5)
MP***	INTEGER	The degrees of polynomial used in smoothing of the excitation function data (The default value is 3)
IPRT	INTEGER	The control index for printing of intermediate results of calculation, IPRT = 0 for no printing, = 1 for printing
		--- Output Data ---
PCTF(J)	REAL*8 (20)	The distribution (%) of recoil products in J-th material to the rear of the target foil(The target foil corresponds to J = 1) [J = 1,NFL]
PCTB(J)	REAL*8 (20)	The distribution (%) of recoil products in J-th material to the front of the target foil

Table 10 continued

		(The target foil corresponds to J = 1) [J = 1,NFL]
EIN(M)	REAL*8 (0:15)	The mean projectile energy (MeV) in M-th divided target (The initial projectile energy corresponds to M=0) [M = 0,NTGT]
TGS(M)	REAL*8 (15)	The thickness (mg/cm^2) of M-th divided target from the front [M = 1,NTGT]

* Ejectiles can be specified up to three types. For example, the ejectiles in the reaction system: ^{197}Au(^{16}O, α p2n)^{206}Pb is specified as

N4(1) = 1, N4(2) = 1, N4(3) = 2,
IZ4(1) = 2, IZ4(2) = 1, IZ4(3) = 0,
IA4(1) = 4, IA4(2) = 1, IA4(3) = 1

** This value can be obtained from SUBROUTINE ELMDA3 (cf.Section 4.8)

*** To obtain the smoothing cross section at a given projectile energy, the excitation function data are fitted by MP-degree polynomial for NP data centered in the energy.

Table 11 Arguments of SUBROUTINE DATSIG

Variable Name	Format	Remark
		--- Input data ---
IW	INTEGER	The unit specifier for printing of final results of calculation

Table 12 List of block common in SUBROUTINE ELMDA3

Variable Name	Format	Remark
ELN	CHARACTER*2	Elemental symbol
ATW	REAL*8	Atomic weight
DSTY	REAL*8	Solid density (g/cm^3)
FRMV	REAL*8	The Fermi velocity of solid, in units of the Bohr velocity[3]
FSCR	REAL*8	Factor determining ion screening length[3]
COFP	REAL*8	Proton stopping cross section coefficients[3]
X0	REAL*8	The parameter used in calculation of the density correction for stopping powers[8]
X1	REAL*8	The parameter of density correction[8]
AA	REAL*8	The parameter of density correction[8]
AM	REAL*8	The parameter of density correction[8]
D0	REAL*8	The parameter of density correction[8]
POT	REAL*8	The mean excitation potential (eV) of orbital electrons in the target element.[8]

Table 13 Job control statements for BATCH processing

```
// JCLG JOB
// EXEC JCLG
// SYSIN DD DATA,DLM='++'
// ····  JUSER statement  ····
   C.00 I.00 T.00 W.00
   OPTP PASSWORD=XXXXXXXX
// EXEC LMGO,LM='JXXXX.OSCAR3B'
// EXPAND DISKTO,DDN=FT01F001,DSN='JXXXX.MASWPS'
// EXPAND DISKTO,DDN=FT03F001,DSN='JXXXX.OSIO',
   Q='.DATA(OPTB)'
// SYSIN DD *


         ····  Input Data Set  ····

++
//
```

Table 14 Input format of BATCH processing
(The symbol D represents default value. All projectile energies is in the laboratory system)

Format of 1st line: Kinds of calculation

Variable Name	Format	Column Used	Remark
ICAL*	I1	1	The control index for kinds of calculation, ICAL=1: Calculation of the yield of radioisotopes, =2: Calculation of the energy loss in the stacked target, =3: Calculation of stopping powers and projected ranges, =4: Calculation of the distribution of recoil products in the stacked target, =0: Termination
IW	I4	2-5	The unit specifier for output (D = 6).

* The format of next lines vary with this value.

Table 14 continued

ICAL = 1: Calculation of the yield of radioisotopes (1)

The samples of I/O are shown in Table 15.

Formats of 2nd line: Comment line

Variable Name	Format	Column Used	Remark
COM	A60	1-60	Comments

Format of 3rd line: Reaction system

Variable Name	Format	Column Used	Remark
IZ1	I5	1-5	Projectile atomic number
IA1	I5	6-10	Projectile mass number
KZ2	I5	11-15	Target atomic number
KA2	I5	16-20	Target mass number
IZ3	I5	21-25	Product atomic number
IA3	I5	26-30	Product mass number
N4(1)*	I3	31-33	The number of 1st-ejectiles
IZ4(1)	I3	34-36	1st-ejectile atomic number
IA4(1)	I3	37-39	1st-ejectile mass number
N4(2)	I3	40-42	The number of 2nd-ejectiles
IZ4(2)	I3	43-45	2nd-ejectile atomic number
IA4(2)	I3	46-48	2nd-ejectile mass number
N4(3)	I3	49-51	The number of 3rd-ejectiles
IZ4(3)	I3	52-54	3rd-ejectile atomic number
IA4(3)	I3	55-57	3rd-ejectile mass number

* Ejectiles can be specified up to three types. For example, the ejectiles in the reaction system: $^{197}Au(^{16}O, \alpha\ p2n)^{206}Pb$ is specified as

N4(1) = 1, N4(2) = 1, N4(3) = 2,
IZ4(1) = 2, IZ4(2) = 1, IZ4(3) = 0,
IA4(1) = 4, IA4(2) = 1, IA4(3) = 1

Table 14 continued

ICAL = 1: Calculation of the yield of radioisotopes (2)

Formats of 4th line: Target, product and excitation function

Variable Name	Format	Column Used	Remark
IZ2(1)*	I5	1-5	Target atomic number
A2(1)	F5.1	6-10	Target atomic weight (D : The value is obtained from SUBROUTINE ELMDA3)
NEL(1)	I5	11-15	When the target material is composed of mono-atoms, this value is 1. When the material is composed of different atomic species, this value is the composition ratio of the target element in the compound(D = 1)
NKD	I5	16-20	The number of kinds of elements in the target material (D = 1)
TD	F5.1	21-25	The thickness(mg/cm^2) of target material (D = 0), TGD = 0 for calculation of thick-target yields, = -TGD for calculation of thin-target yields**
ISIG	I5	26-30	The control index for input of the excitation function data (D = 0), ISIG = 0 for arranging input data,

Table 14 continued

			= 1 for calculating the excitation function using the empirical rule.
NEX	I5	31-35	The number of cross sections in the excitation function data (D = 0)
THALF	F10.4	36-45	The half-life of product nuclei
THUNIT	A3,2X	46-48	The unit of half-lives (D = 'HR '), THUNIT = 'SEC': Units in second, = 'MIN': Units in minute, = 'HR ': Units in hour, = 'DAY': Units in day, = 'YR ': Units in year
ABDC	F10.4	51-60	The abandonce of the target nuclide (D = 1)
MP***	I5	61-65	The degrees of polynomial used in smoothing of the excitation function data (D = 3)
NP***	I5	66-70	The number of smoothing points (D = 5)
IPRT	I1	71	The control index for printing of intermediate results of calculation of the excitation function,

Table 14 continued

				IPRT = 0 for no printing, = 1 for printing

* If the target material is composed of different atomic species, the target element is to be specified at the beginning of the array.

** It is assumed that the yield is proportional to the thickness of the target material.

*** To obtain the smooting cross section at a given projectile energy, the excitation function data are fitted by MP-degree polynomial for NP data centered in the energy.

Table 14 continued

ICAL = 1: Calculation of the yield of radioisotopes (3)

If the target material is composed of diffrent atomic species (NKD > 1), the following input data are added by (NKD -1) lines

Variable Name	Format	Column Used	Remark
IZ2(I)*	I5	1-5	The atomic number of I-th element
A2(I)	F5.1	6-10	The atomic weight of I-th element (D : the value is obtained from SUBROUTINE ELMDA3)
NEL(I)	I5	11-15	The composition ratio of I-th element (D = 1)

* I = 2,NKD

Table 14 continued

ICAL = 1: Calculation of the yield of radioisotopes (4)

Format of 5 + (NKD - 1) line: Incident energy and irradiation time

Variable Name	Format	Column Used	Remark
EA	F10.3	1-10	Projectile energy. When a user wish to calculate the yields for the energies more than one, EA is the initial energy. When ISIG is 1, EA is 0
EZ	F10.3	11-20	When a user wish to calculate the yields for energies more than one, EZ is the final energy (D = 0)
DE	F10.3	21-30	When a user wish to calculate the yields for energies more than one, DE is the increment of the energy (D = 0)
EUNIT	A3,2X	31-33	The unit of the incident energy (D = 'MEV'), EUNIT = 'MEV': Units in MeV, = 'M/A': Units in MeV/amu
TA	F10.3	36-45	Irradiation time. When a user wish to calculate the yields for the times more than one, TA is the initial time

Table 14 continued

TZ	F10.3	46-55	When a user wish to calcu-ate the yields for times more than one, TZ is the final energy (D = 0)
TE	F10.3	56-65	When a user wish to calcu-late the yields for times more than one, TE is the increment of the time (D = 0)
TMUNIT	A3	66-68	The unit of irradiation times (D = 'HR '), TMUNIT = 'SEC': Units in second, = 'MIN': Units in minute, = 'HR ': Units in hour, = 'DAY': Units in day, = 'YR ': Units in year

If ISIG is 0, following input data are added by NEX lines

Variable Name	Format	Column Used	Remark
EEX(I)*	F10.5	1-10	Projectile energy (MeV)
CRS(I)	F10.5	11-20	Cross section (mb)

* I = 1,NEX

Table 14 continued

ICAL = 2: Calculation of the energy loss in the stacked target (1)
The samples of I/O are shown in Table 16.

Format of 2nd line: Comment line

Variable Name	Format	Column Used	Remark
COM	A60	1-60	Comments

Format of 3rd line: Projectile and target

Variable Name	Format	Column Used	Remark
IZ1	I5	1-5	Projectile atomic number
IA1	I5	6-10	Projectile mass number
ENG	F10.3	11-20	Projectile energy
EUNIT	A3,2x	21-23	The unit of the energy (D = 'MEV'), EUNIT = 'MEV': Units in MeV, = 'M/A': Units in MeV/amu
NTG	I5	26-30	The number of the materials in the stacked target

Table 14 continued

ICAL = 2: Calculation of the energy loss in the stacked target (2)

The following input data are added by NTG lines.

Variable Name	Format	Column Used	Remark
IIZ2(I,1)*	I5	1-5	The atomic number of 1st element in I-th stacked target
AA2(I,1)	F5.1	6-10	The atomic weight of 1st element (D : the value is obtained from SUBROUTINE ELMDA3)
NNEL(I,1)	I5	11-15	When I-th target material is composed of mono-atoms, the value is 1. When the material is composed of different atomic species, this value is the composition ratio of 1st element in the compound (D = 1)
NNKD(I)	I5	16-20	The number of kinds of elements in I-th material (D = 1)
TD(I)	F10.2	21-30	The thickness (mg/cm^2) of I-th material
COMT(I)	A10	31-40	The comment for I-th material.

* I = 1,NTG

Table 14 continued

If I-th material is composed of different atomic species (NNKD(I) > 1), the following input data are added by (NNKD(I) - 1) lines

Variable Name	Format	Column Used	Remark
IIZ2(I,J)*	I5	1-5	The atomic number of J-th element in I-th stacked target
AA2(I,J)	F5.1	6-10	The atomic weight of J-th element (D : The value is obtained from SUBROUTINE ELMDA3)
NNEL(I,J)	I5	11-15	When I-th target material is composed of mono-atoms, the value is 1. When the material is composed of different atomic species, this value is composition ratio of J-th element in the compound(D=1)

* J = 2,NNKD(I)

Table 14 continued

ICAL = 3: Calculation of stopping powers and projected ranges (1)

The samples of I/O are shown in Table 17.

Format of 2nd line: Comment line

Variable Name	Format	Column Used	Remark
COM	A60	1-60	Comments

Format of 3rd line: Projectile and units

Variable Name	Format	Column Used	Remark
IZ1	I5	1-5	Projectile atomic number
IA1	I5	6-10	Projectile mass number
IUNS	I5	11-15	Index for the unit of stopping powers (D = 0), IUNS = 0: Units in MeV/(mg/cm^2), = 1: Units in eV/(10^{15}atoms/cm^2)
IUNR	I5	16-20	Index for the unit in ranges (D = 0), IUNR = 0: Units in mg/cm^2, = 1: Units in μm

Table 14 continued

ICAL = 3: Calculation of stopping powers and projected ranges (2)

format of 4th line: Target

Variable Name	Format	Column Used	Remark
IZ2(1)	I5	1-5	The atomic number of 1st element in the target material
A2(1)	F5.1	6-10	The atomic weight of 1st element (D : the value is obtained from SUBROUTINE ELMDA3)
NEL(1)	I5	11-15	When the target material is composed of mono-atoms, the value is 1. When the material is composed of different atomic species, this value is the composition ratio of 1st element in the compound (D = 1)
NKD	I5	16-20	The number of kinds of elements in the material(D = 1)
DSTT	F10.4	21-30	The density (g/cm^3) of the compound target (D = 0)

Table 14 continued

If the target material is composed of different atomic species (NKD > 1), following input data are added by (NKD - 1) lines

Variable Name	Format	Column Used	Remark
IZ2(I)*	I5	1-5	The atomic number of I-th element in the material
A2(I)	F5.1	6-10	The atomic weight of I-th element (D : the value is obtained from SUBROUTINE ELMDA3)
NEL(I)	I5	11-15	The composition ratio of I-th element in the material (D = 1)

* I = 2,NKD

Table 14 continued

ICAL = 3: Calculation of stopping powers and projected ranges (3)

format of 5 + (NKD -1) line: Projectile energy

Variable Name	Format	Column Used	Remark
EA	F10.3	1-10	Projectile energy. When a user wish to calculate the stopping powers and projected ranges for the energies more than one, EA is the initial energy
EZ	F10.3	11-20	When a user wish to calculate those for energies more than one, EZ is the final energy (D = 0)
DE	F10.3	21-30	When a user wish to calculate those for energies more than one, DE is increment of the energy (D = 0)
EUNIT	A3	31-33	The unit of the energy, EUNIT = 'MEV': Units in MeV, = 'M/A': Units in MeV/amu

Table 14 continued

ICAL = 4: Calculation of the distribution of recoil products in the stacked target (1)

The samples of I/O are shown in Table 18.

Format of 2nd line: Comment line

Variable Name	Format	Column Used	Remark
COM	A60	1-60	Coments

Format of 3rd line: Reaction mechanism, target and excitation function

Variable Name	Format	Column Used	Remark
IRCT	I5	1-5	Control index for reaction mechanism, IRCT = 0: Evaporation process from compound nuclei assuming full momentum transfer = 1: Symmetric fission process = 2: Asymmetric fission process
NFL	I5	6-10	The number of constituent materials of the stacked target

Table 14 continued

ITG	I5	11-15	The order of the material which contains target nuclides in the stacked target. The material faced on incident beams is specified as ITG = 1 (D = 1)
NTGT	I5	16-20	The number of dividing of the material which contains target nuclides (D = 1) (cf. Section 2.4)
IPRT	I5	21-25	The control index for printing of intermediate results of calculation, IPRT = 0 for no printing, = 1 for printing
MP*	I5	26-30	The degrees of polynomial used in smoothing of the excitation function data (D = 3)
NP*	I5	31-35	The number of smoothing points (D = 5)
NEX**	I5	36-40	The number of cross sections in the excitation function data

* To obtain the smooting cross section at a given projectile energy, the excitation function data are fitted by MP-degree polynomial for NP data centered in the energy.

** The excitation function must be taken into consideration at calculation of the distribution of the recoil products when the energy loss of the ions in the target foil is large so that the variation of cross sections in the target is not negligibly small.

Table 14 continued

ICAL = 4: Calculation of the distribution of recoil products in the stacked target (2)

Format of 4th line: Projectile energy, Q-value and scattering angle

Variable Name	Format	Column Used	Remark
E1L	F10.3	1-10	Projectile energy (MeV)
Q	F10.3	11-20	Reaction Q-value (MeV). If Q is 0, it is calculated as Q_{gg}-value using the Wapstra's mass data for IRCT = 0 or is calculated from the kinetic energy of fission products for IRCT = = 1 and 2 (D = 0)
NANG*	I5	21-25	The number of dividing of π radian in the CM system (D = 100)
ANS1**	F10.3	26-35	Anisotropy coefficient in angular distribution of fission products (D = 0)

* NANG corresponds to N_g in Eq.(25)

** ANS1 corresponds to a in Eq.(24)

Table 14 continued

Format of 5th line: Reaction system

Variable Name	Format	Column Used	Remark
IZ1	I5	1-5	Projectile atomic number
IA1	I5	6-10	Projectile mass number
IZ2	I5	11-15	Target atomic number
IA2	I5	16-20	Target mass number
IZ3	I5	21-25	Product atomic number
IA3	I5	26-30	Product mass number
N4(1)*	I3	31-33	The number of 1st-ejectiles
IZ4(1)	I3	34-36	1st-ejectile atomic number
IA4(1)	I3	37-39	1st-ejectile mass number
N4(2)	I3	40-42	The number of 2nd-ejectiles
IZ4(2)	I3	43-45	2nd-ejectile atomic number
IA4(2)	I3	46-48	2nd-ejectile mass number
N4(3)	I3	49-51	The number of 3rd-ejectiles
IZ4(3)	I3	52-54	3rd-ejectile atomic number
IA4(3)	I3	55-57	3rd-ejectile mass number

* Ejectiles can be specified up to three types. For example, the ejectiles in the reaction system:
$^{197}Au(^{16}O, \alpha\, p2n)^{206}Pb$ is specified as

N4(1) = 1, N4(2) = 1, N4(3) = 2,
IZ4(1) = 2, IZ4(2) = 1, IZ4(3) = 0,
IA4(1) = 4, IA4(2) = 1, IA4(3) = 1

Table 14 continued

ICAL = 4: Calculation of the distribution of recoil products in the stacked target (3)

The following input data are added by NFL lines.

Variable Name	Format	Column Used	Remark
COMT(I)*	A10	1-10	The comment line for I-th material
JZ2(I,1)	I5	11-15	The atomic number of 1st element in I-th material
AA2(I,1)	F5.1	16-20	The atomic weight of 1st element (D : the value is obtained from SUBROUTINE ELMDA3)
NEL(I,1)	I5	21-25	When I-th target material is composed of mono-atoms, the value is 1. When the material is composed of different atomic species, this value is the composition ratio of 1st element in the compound (D = 1)
TGD(I)	F10.3	26-35	The thickness (mg/cm^2) of I-th material
NKD(I)	I5	36-40	The number of kinds of the element in I-th material (D = 1)

* I = 1, NFL

Table 14 continued

If I-th material is composed of different atomic species (NKD(I) > 1), the following input data are added by (NKD(I) - 1) lines

Variable Name	Format	Column Used	Remark
JZ2(I,J)*	10X,I5	11-15	The atomic number of J-th element in I-th material
AA2(I,J)	F5.1	16-20	The atomic weight of J-th element (D = the value is obtained from SUBROUTINE ELMDA3)
NEL(I,J)	I5	21-25	The composition ratio of J-th element in I-th material (D = 1)

* J = 2, NKD(I)

If NEX is over 0, following input data are added by NEX lines

Variable Name	Format	Column Used	Remark
EEX(I)	F10.5	1-10	Projectile energy (MeV)
CRS(I)	F10.5	11-20	Cross section (mb)

Table 15 Sample of the input data for calculation of the yield of radioisotopes

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
1
TEST RUN
    3    7    83  209    86  211    5  0  1
  83209.       1    1          1414.2
46.      48.       1.              1.       2.       1.
  38.30000   0.10000
  40.10000   0.80000
  40.70000   2.40000
  42.20000   8.60000
  42.20000  11.60000
  43.00000  36.30000
  43.30000  38.20000
  44.00000  55.90000
  45.10000 120.00000
  45.20000 136.00000
  45.80000 190.00000
  47.00000 220.00000
  47.40000 301.00000
  48.80000 431.00000
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
```

Sample of the output for the input data
(CPU time = 0.13 s)

```
DATE : 88-05-06                     FINAL RESULTS
*****************************************************************
TITLE ==> TEST RUN

PRODUCTION YIELDS FOR LI-  7 + BI-209.00000 * 1 --> RN-211
*****************************************************************

THICK-TARGET IS USED.
EXCITATION FUNCTION WAS GIVEN FROM INPUT DATA.

HALF LIFE OF PRODUCT =     14.200 HR
ABUNDANCE OF TARGET NUCLIDE = 1.0000
DEGREE OF POLYNOMIAL  IN SMOOTHING =  3
NUMBER OF DATA POINTS IN SMOOTHING =  5

INCIDENT ENERGY    = 4.60000D+01 MEV
SATURATION FACTOR = 2.22803D+02 MC/MA

IRRAD.TIME :     YIELD   :
     (HR ) :    (MC/MA)  :
 1.0000D+00  1.0615D+01
 2.0000D+00  2.0723D+01

INCIDENT ENERGY    = 4.70000D+01 MEV
SATURATION FACTOR = 3.85183D+02 MC/MA

IRRAD.TIME :     YIELD   :
     (HR ) :    (MC/MA)  :
 1.0000D+00  1.8350D+01
 2.0000D+00  3.5827D+01

INCIDENT ENERGY    = 4.80000D+01 MEV
SATURATION FACTOR = 6.09418D+02 MC/MA

IRRAD.TIME :     YIELD   :
     (HR ) :    (MC/MA)  :
 1.0000D+00  2.9033D+01
 2.0000D+00  5.6683D+01
---------------------------------------
```

Table 16 Sample of the input data for calculation of the energy loss in stacked targets

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
2
TEST RUN
    1    1 30.                 3
   42               24.        MO
   29               78.        CU
   13        2    2 128.       AL2O3
    8        3
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
```

Sample of the output for the input data
(CPU time = 0.35 s)

```
DATE : 88-05-06                   FINAL RESULTS
*******************************************************************************
TITLE ==> TEST RUN

ENERGY LOSS FOR PROJECTILE H-  1
*******************************************************************************

E1 = INCIDENT ENERGY, DE = ENERGY LOSS, RE = RESIDUAL ENERGY
```

STACK			THICK. (MG/CM2)	E1 (MEV)	DE (MEV)	RE (MEV)
1 MO	95.94000 * 1	MO	2.4000D+01	3.0000D+01	2.6367D-01	2.9736D+01
2 CU	63.53999 * 1	CU	7.8000D+01	2.9736D+01	9.5830D-01	2.8778D+01
3 AL O	26.98100 * 2 15.99900 * 3	AL2O3	1.2800D+02	2.8778D+01	2.0235D+00	2.6755D+01

Table 17 Sample of the input data for calculation of stopping powers and projected ranges

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
3
TEST RUN
    8    16
   79
.002          .01         .002        M/A
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
```

Sample of the output for the input data
(CPU time = 0.15 s)

```
DATE : 88-05-06                  FINAL RESULTS
******************************************************************************
TITLE ==> TEST RUN

STOPPING POWER AND RANGE FOR  O- 16 IN AU-196.97000 * 1
******************************************************************************
    ST, SE, SN = TOTAL, ELECTRONIC AND NUCLEAR STOPPING POWER (MEV/MG/CM2)
            RP = PROJECTED RANGE (MG/CM2)
TARGET DENSITY =  1.93110D+01 G/CM3

    ENERGY :     ENERGY :        ST    :         SE   :         SN   :         RP   :
   (MEV/U) :      (MEV) :
--------------------------------------------------------------------------
 2.0000E-03  3.2000E-02  2.2389D-01  1.2441D-01  9.9476D-02  4.0524D-02
 4.0000E-03  6.4000E-02  2.7878D-01  1.8426D-01  9.4518D-02  7.7455D-02
 6.0000E-03  9.6000E-02  3.1485D-01  2.2697D-01  8.7888D-02  1.1561D-01
 8.0000E-03  1.2800E-01  3.4678D-01  2.6498D-01  8.1805D-02  1.5434D-01
 1.0000E-02  1.6000E-01  3.7681D-01  3.0032D-01  7.6495D-02  1.9322D-01
--------------------------------------------------------------------------
```

Table 18 Sample of the input data for calculation of the distribution of recoil products in stacked targets

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
4
TEST RUN
    1    5         3
20.
    1    1        92  235       63  153  1 30 83
AL                13                10.
AL                13                 2.
UO2               92             1   2.         2
                   8             2
AL                13                 2.
AL                13                10.
----+----1----+----2----+----3----+----4----+----5----+----6----+----7--
```

Table 18 continued

Sample of the output for the input data

(CPU time = 29 s)

```
DATE : 88-05-06                 FINAL RESULTS
*******************************************************************
TITLE ==> TEST RUN

DISTRIBUTION OF RECOIL PRODUCTS IN STACKED TARGET
*******************************************************************


       <<<<<  REACTION SYSTEM  >>>>>

              PROJECTILE =  H -   1
                  TARGET =  U - 235
                RESIDUAL = EU - 153
        EMITTED PARTICLES = ZN -  83 *    1

           FIRST COMPOUND = NP - 236


       ASSUMED REACTION TYPE = FISSION
       REACTION Q-VALUE(MEV) =   1.52531D+02


       <<<<<  TABLE ON STACKED TARGET   >>>>>


-----------------------------------------------------------
  1  AL            AL- 26.98100 * 1     1.00000D+01 MG/CM2
-----------------------------------------------------------
  2  AL            AL- 26.98100 * 1     2.00000D+00 MG/CM2
-----------------------------------------------------------
  3  UO2            U-238.03999 * 1     2.00000D+00 MG/CM2
                    O- 15.99900 * 2
-----------------------------------------------------------
  4  AL            AL- 26.98100 * 1     2.00000D+00 MG/CM2
-----------------------------------------------------------
  5  AL            AL- 26.98100 * 1     1.00000D+01 MG/CM2
-----------------------------------------------------------
       <<<<<  PROJECTILE ENERGY DISTRIBUTION IN TARGET  >>>>>

             INITIAL PROJECTILE ENRGY(MEV) =  2.00000D+01

          PASS LENGTH     PROJECTILE ENG  PROJECTILE ENG
            (MG/CM2)        (MEV-LAB)        (MEV-CMS)
      ---------------------------------------------------
       1  1.00000D+00      1.97467D+01      1.96630D+01
      ---------------------------------------------------
        <<<<<  DISTRIBUTION OF RECOIL PRODUCTS IN STACKED TAGETS  >>

           NUMBER OF DIVIDING ANGLE   = 100
          NUMBER OF DIVIDING TARGET   =   1
         ANISOTROPY COEFFICIENT       =   0.0
                    LOSS OF RESIDUE   =   0.0          %

         STACKED TARGET   FOWARD (%)    BKWARD (%)     TOTAL (%)
       -----------------------------------------------------------
         1  AL            0.0           6.96289D+00  6.96289D+00
         2  AL            0.0           3.36680D+01  3.36680D+01
         3  UO2           7.83720D+00   7.79853D+00  1.56357D+01
         4  AL            3.41842D+01   0.0          3.41842D+01
         5  AL            9.54915D+00   0.0          9.54915D+00
       -----------------------------------------------------------
```

Table 19 Command procedure in TSSMAC.CLIST(OT) for TSS processing

```
PROC 0
CONTROL NOF MA
ALLOC DA(MASWPS.DATA) F(FT01F001) SHR
ALLOC DA(OSIO.DATA(OPTT)) F(FT10F001) SHR
ALLOC DA(OSIO.DATA(IPT1)) F(FT11F001) SHR
ALLOC DA(OSIO.DATA(IPT2)) F(FT12F001) SHR
ALLOC DA(OSIO.DATA(IPT3)) F(FT13F001) SHR
ALLOC DA(OSIO.DATA(IPT4)) F(FT14F001) SHR
CALL OSCAR3T
EXIT
```

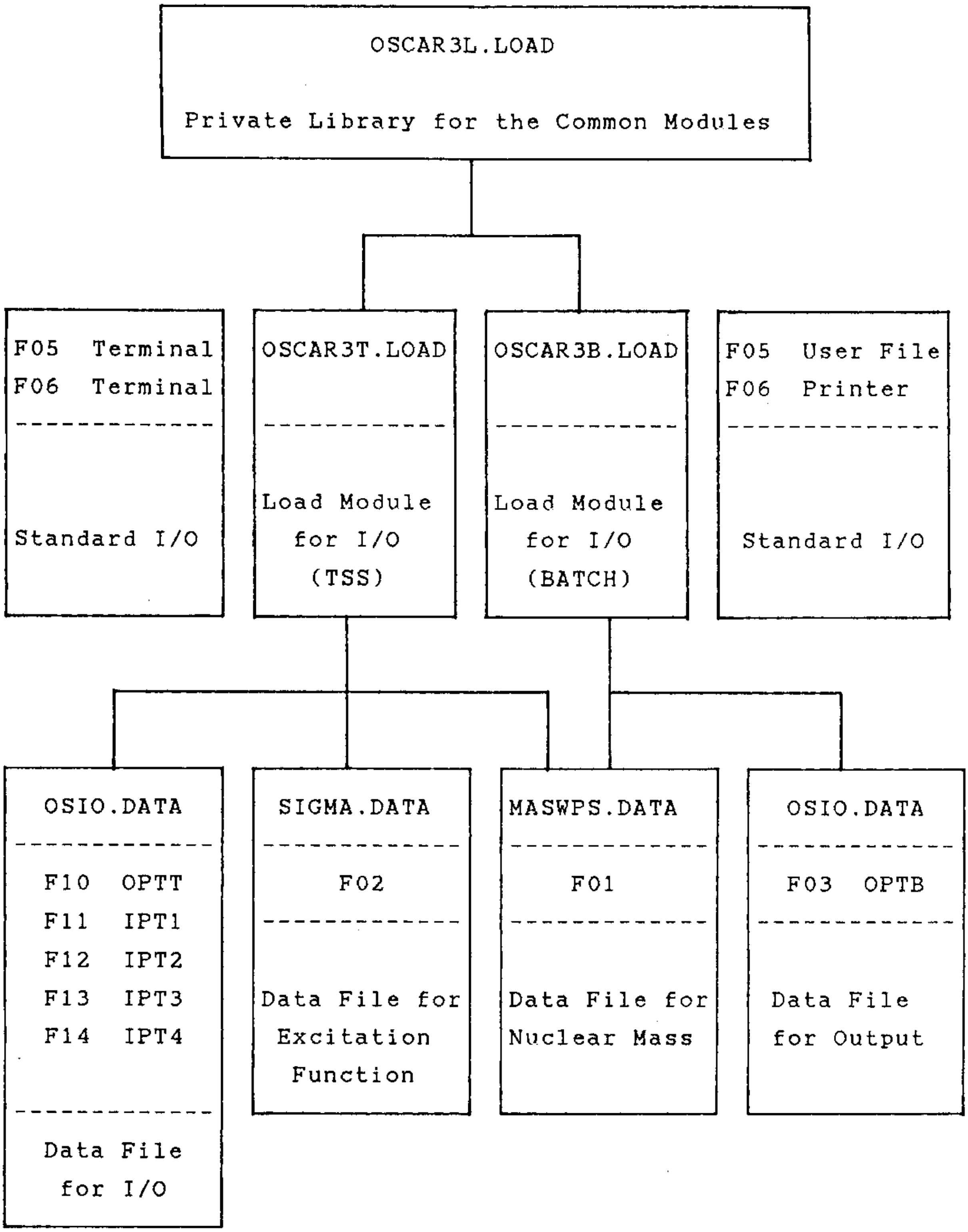

Fig.1 Structure of load modules and data files

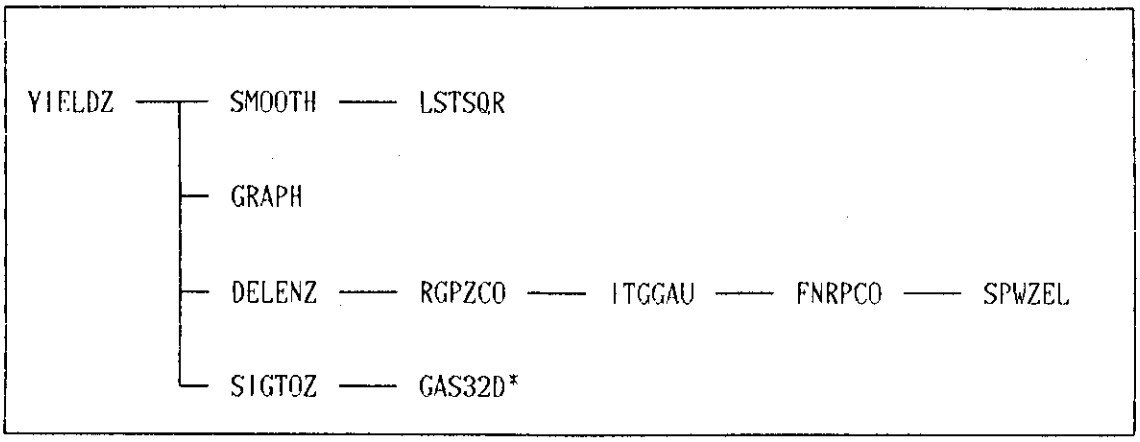

Fig.2 Tree structure of subprograms in SUBROUTINE YIELDZ
Intrinsic functions used in the subroutine were omitted from this figure
* This subprogram is the double precision function in the scientific subroutine library of FACOM which evluates the integrated value of function f(x) in a given region using Gauss-Legendre method.

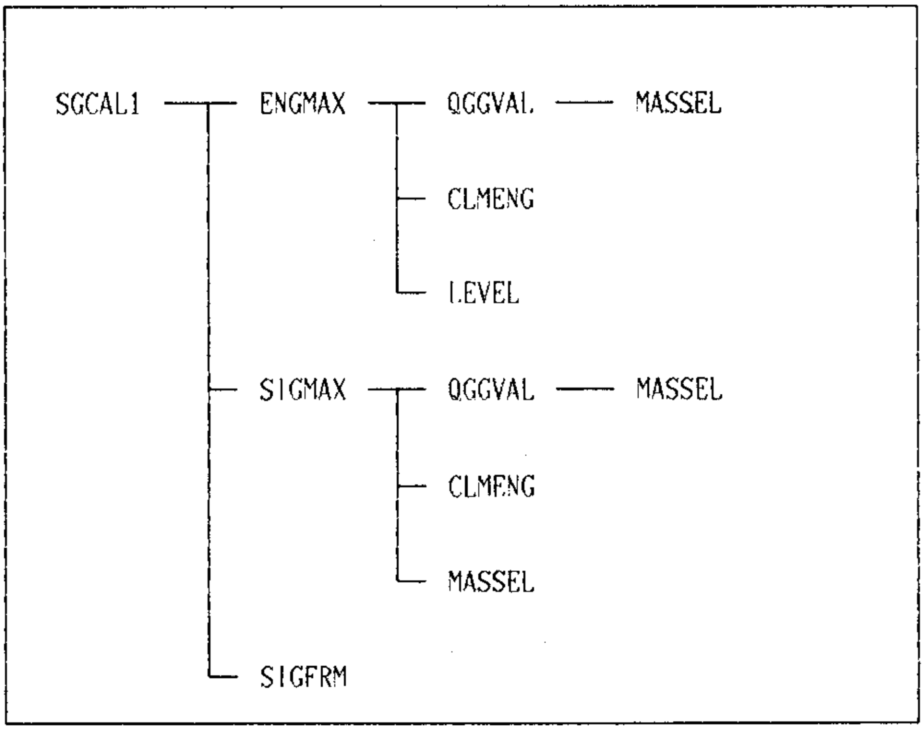

Fig.3 Tree structure of subprograms in SUBROUTINE SGCAL1
Intrinsic functions used in the subroutine were omitted from this figure

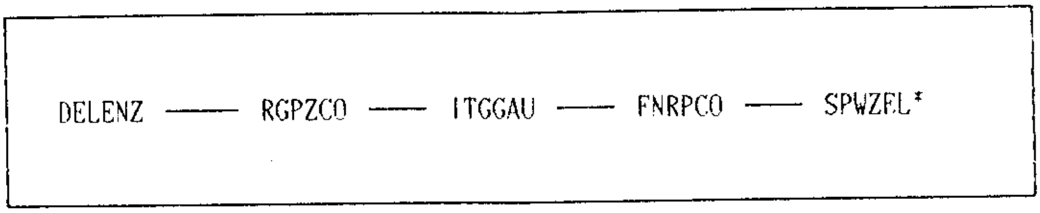

Fig.4 Tree structure of subprograms in DOUBLE PRECISION FUNCTION DELENZ
Intrinsic functions used in the subroutine were omitted from this figure
* cf. Fig.5

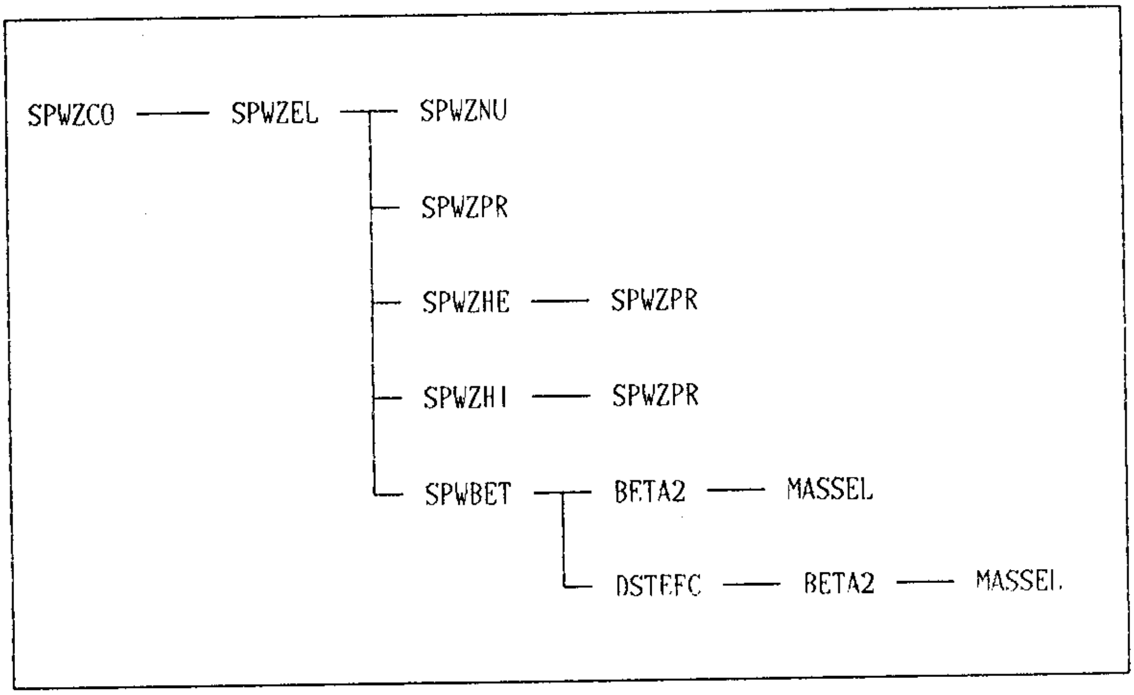

Fig.5 Tree structure of subprograms in SUBROUTINE SPWZCO
Intrinsic functions used in the subroutine were omitted from this figure

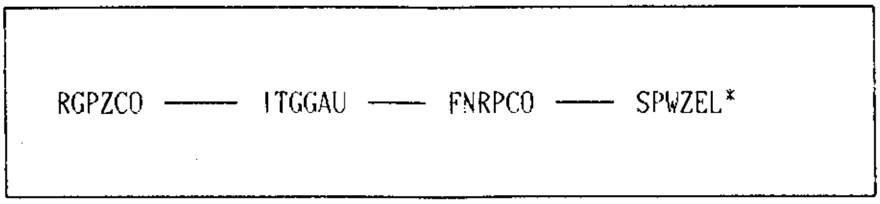

Fig.6 Tree structure of subprograms in DOUBLE PRECISION FUNCTION RGPZCO
Intrinsic functions used in the subroutine were omitted from this figure
* cf. Fig.5

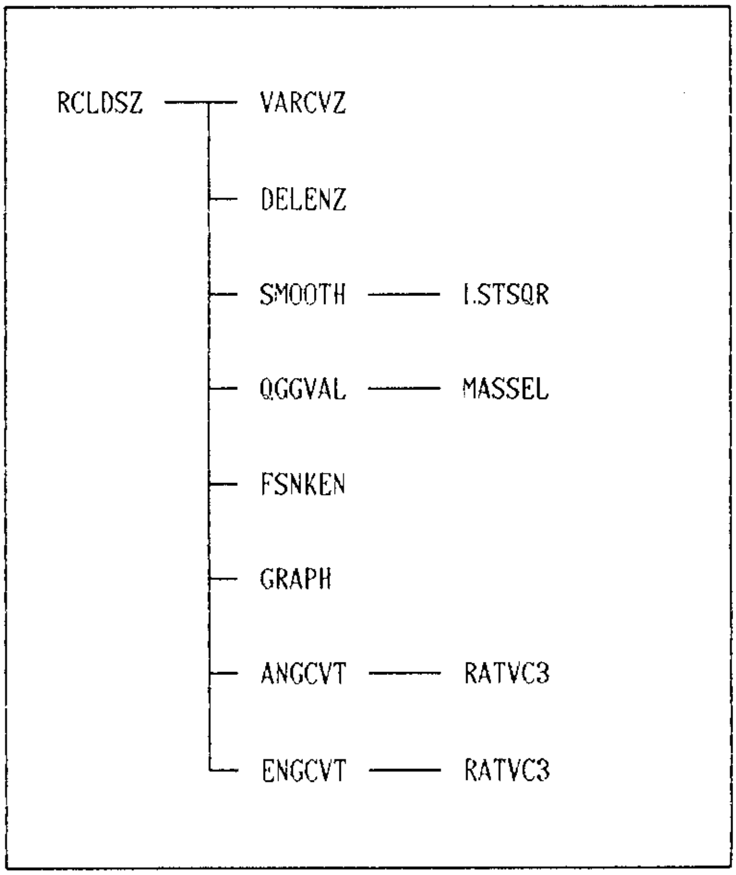

Fig.7 Tree structure of subprograms in SUBROUTINE RCLDSZ
Intrinsic functions used in the subroutine were omitted from this figure

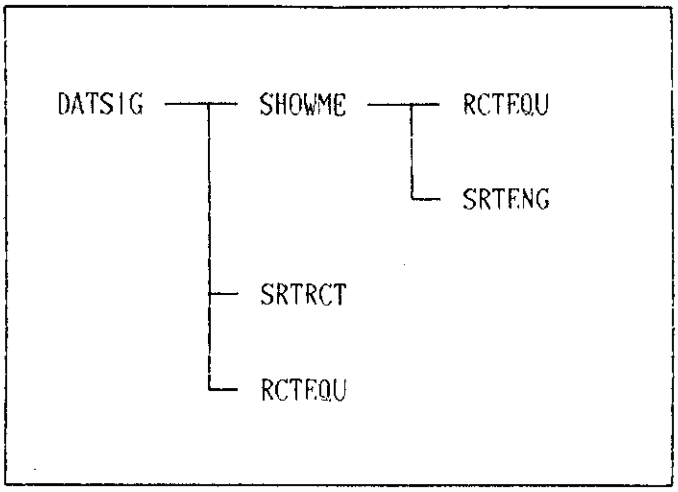

Fig.8 Tree structure of subprograms in SUBROUTINE DATSIG
Intrinsic functions used in the subroutine were omitted from this figure

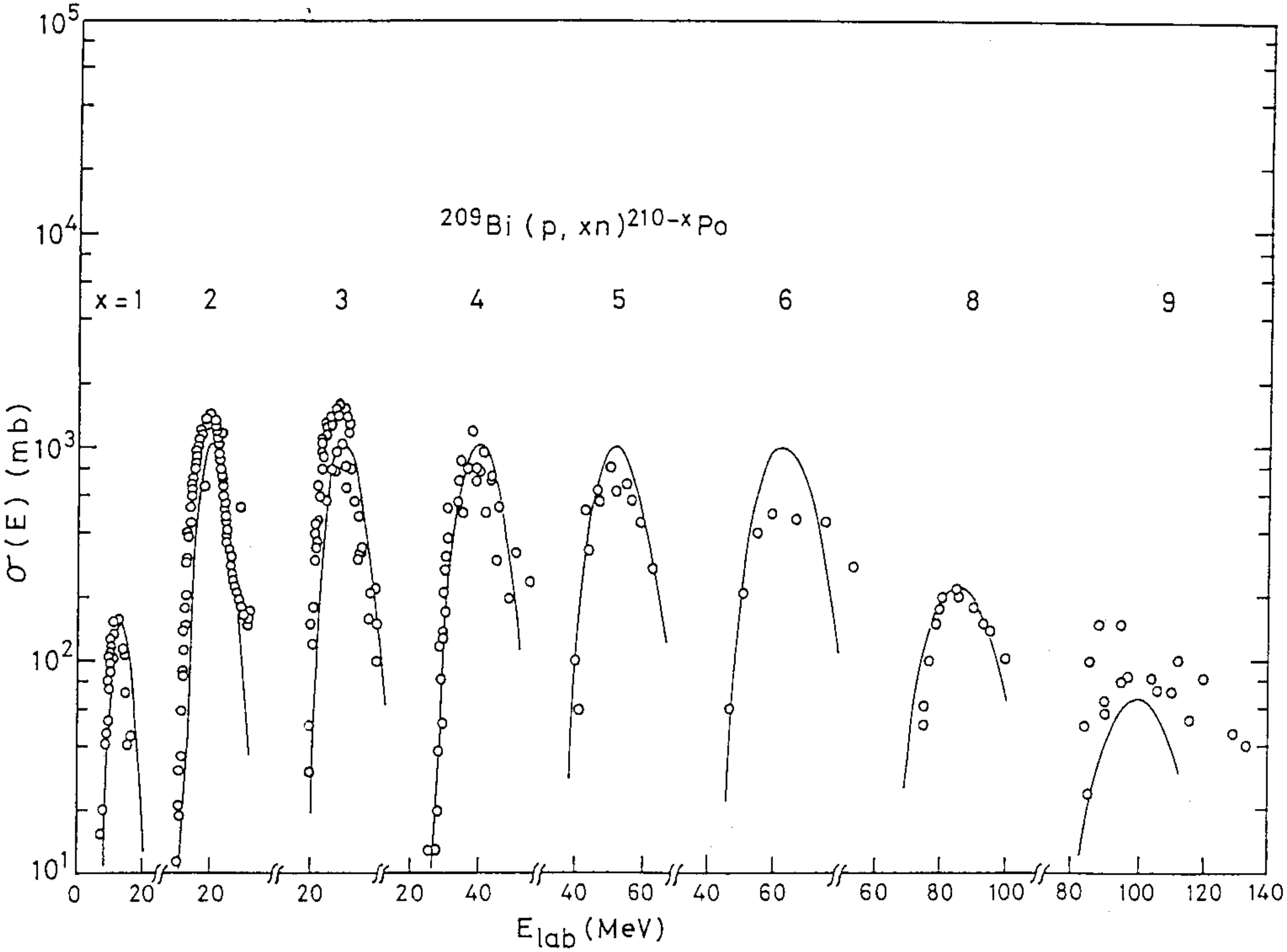

Fig.9 Comparison between calculated (solid line) and experimental values (open circle)[10-17] of the excitation functions for ^{209}Bi(p,xn) reactions

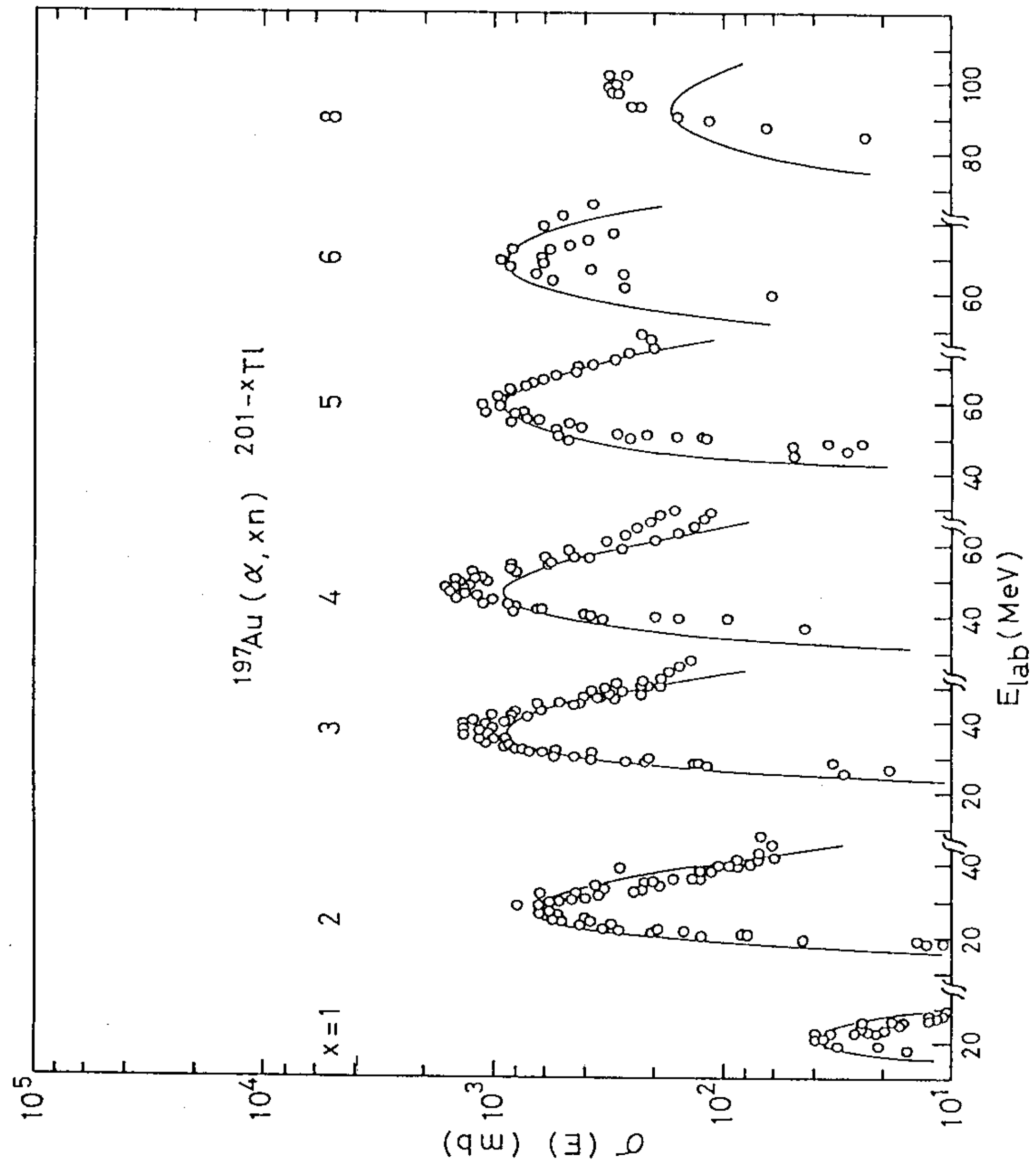

Fig.10 Comparison between calculated (solid line) and experimental values (open circle)[18-21] of the excitation functions for ^{197}Au(α,xn) reactions

Appendix 1

Calculation of Stopping Powers

The basic theory of the energy loss was attempted by Bohr[24] for the first time in a unified fashion, and Bethe[25,26,27] and Bloch[28,29] have derived the fundamental equations for the stopping of very fast particles in a quantized electron plasma in the Born approximation, which are known as Bethe-Bloch equations[9]. The discovery of nuclear fission in the late 1930's evoked a renewed interest in energy loss which brought about a program how to treat the interaction of a partially stripped heavy ion. It was hoped then that, if a degree of ionization of the projectile could be evaluated, the traditional stopping power theories could be applied. Bohr gave a prescription[30] for estimating the effective charge using the Thomas-Fermi atom with a postulate that the ion be considered to be stripped of all electrons with velocities lower than the ion velocity, while Lamb[31] had considered the same problem as Bohr, giving a similar effective charge approximation based on the energy rather than the velocity of the orbital electrons. Then it was successfully attempted by Knipp and Teller[32] to scale the hydrogen stopping powers to those of equivalent helium ions by applying the effective charge concept of Lamb and Bohr. A significant progress has been achieved for the stopping power problem by Northcliffe et al.[33] who unified a wide variety of experimental data by dividing them by the stopping power of protons with the same velocity in the same target. In perturbation theory this ratio should scale as $(Z^*)^2$ where Z^* is the number of electrons left on the ion, and he found a large amount of data could be well described with a simple equation for Z^* containing only two adjustable parameters.

During the 1950's and thereafter there have been fundamental works evaluating both the energy transfer from slow particles to quantized electron plasma and to target nuclei.

Above all, Lindhard and his coworkers[34,35] made an approach concentrating on non-relativistic particle interactions with a free electron gas. The theory worked out by Lindhard et al.[35] has been widely cited as the LSS theory in the literature as one of the first unified theories of ion penetration of solids. It has been widely used as the basis for calculating the electronic stopping of ions in matter. The LSS theory provides a unified approach to the stopping of low energy heavy ions. With this approach, most stopping powers could be estimated within a factor of 2 or 3. The recent use of computers allowed us the incorporation of more realistic Hartree-Fock atom into the theory and gave significant improvement.

Extensive compilations of stopping power measurements have been performed by various authors in the three decades to deduce universal formalisms for different projectile-target combinations. Ziegler et al.[3] have carried out the exhaustive data analysis for protons, alpha-particles and heavy ions in all elements and presented a semi-empirical rule for stopping power calculation with average accuracy of better than 10 % for medium energy heavy ions, and to better than 2 % for high velocity light ions.

In OSCAR, the electronic stopping power is calculated using the Ziegler's formalism at energies below 100 MeV/amu and the Bethe-Bloch formula at energies above 100 MeV/amu. The nuclear stopping power is evaluated using the Ziegler's formula and the total stopping power is obtained by adding both the stopping powers.

1.1 Electronic Stopping Power for Protons[3]

The electronic stopping powers($MeV/(mg/cm^2)$) for protons in a solid target at energies below 100 MeV/amu are expressed as

$$S_p = [1/(1/S_L + 1/S_H)]\cdot 0.6022/M_2, \qquad (1.1)$$

with

$$S_L = aE^b + cE^d, \qquad (1.2)$$

and

$$S_H = e \cdot \ln(g/E + hE)/E^f, \qquad (1.3)$$

where M_2 is the atomic weight of the target element and E proton energy(keV). The parameters from a to h have been determined for all elements by Ziegler.

1.2 Electronic Stopping Power for Alpha-Particles[3)]

The electronic stopping powers(MeV/(mg/cm^2)) for alpha-particles in the solid target at energies below 100 MeV/amu are given by

$$S_{He} = 4\gamma_{He}^2 S_p \qquad (1.4)$$

with

$$\gamma_{He}^2 = 1 - \exp[-\sum_{i=0}^{5} a_i \cdot \ln(E)^i], \qquad (1.5)$$

where γ_{He} is the effective charge coefficient for alpha-particles and E the alpha-particle energy (keV/amu). The parameters a_i were determined by fitting experimental data to Eq.(1.4):

$$\begin{cases} a_0 = 0.2865, & a_1 = 0.1266, & a_2 = -0.001429, \\ a_3 = 0.02402, & a_4 = -0.01135, & a_5 = 0.001475 \end{cases}$$

1.3 Electronic Stopping Power for Heavy Ions[3)]

The electronic stopping powers(MeV/(mg/cm^2)) for heavy ions in the solid target at energies below 100 MeV/amu are expressed as

$$S_{HI} = F\gamma^2 Z_{HI}^2 S_p, \qquad (1.6)$$

where γ is the effective charge coefficient for heavy ions, Z_{HI} the nuclear charge of ions and F the term for Z_1^3 effects.

The effective charge coefficient is given by

$$\gamma = q + (1 - q)/2\cdot(V_0/V_F)^2\cdot \ln[1 + (2\Lambda V_F/a_0V_0)^2], \qquad (1.7)$$

where q denotes the fractional ionization of ions. V_F and V_0 are the Fermi and Bohr velocities of electrons, respectively, in the solid target. a_0 is the Bohr radius and Λ the ion screening length. The fractional ionization is expressed as a function of effective ion velocities y_r:

$$q = 1 - \exp(0.803y_r^{0.3} - 1.3167y_r^{0.6} - 0.38157y_r - 0.008983y_r^2), \qquad (1.8)$$

with

$$y_r = V_r/V_0Z_1^{2/3}, \qquad (1.9)$$

where V_r is the relative velocity of ions to orbital electrons in the target as follows;

$$\begin{cases} V_r = V_1(1 + 1/5V_R^2) & \text{for } V_1 \geqq V_F, \quad (1.10) \\ V_r = 3V_F/4\cdot(1 + 2V_R^2/3 - V_R^4/15) & \text{for } V_1 < V_F, \quad (1.11) \end{cases}$$

with

$$V_R = V_1/V_F$$

where V_1 is the ion velocity. The screening length is given by

$$\Lambda = \frac{2a_0(1-q)^{2/3}}{Z_1^{1/3}[1 - (1-q)/7]}, \qquad (1.12)$$

and the term for the Z_1^3 effect is expressed by

$$F = 1 + (0.18 + 0.0015Z_2)/Z_1^2\cdot\exp[-(7.6 - \ln E)^2] \qquad (1.13)$$

Eq.(1.6) is valid for $y_r > 0.13$ or $V_r > 1.0$ of ion velocities. At lower velocities, the electronic stopping power is calculated as to be proportional to ion velocities:

$$S_{HI} = \gamma'^2 Z_1^2 S_p' (E/E')^p, \tag{1.14}$$

with

$$\begin{cases} p = 0.5 & \text{for } Z_1 \geqq 20, \text{ or } Z_2 \neq 6, 14 \text{ and } 32, \\ p = 0.375 & \text{for } Z_1 < 20, \text{ and } Z_2 = 6, 14 \text{ or } 32, \end{cases}$$

where E' denotes the ion kinetic energy at $y_r = 0.13$ or $V_r = 1.0$. γ' and S_p' are the effective charge coefficient and stopping power, respectively, at the energy of E'.

1.4 Electronic Stopping power at energies above 100 MeV/amu[9]

The electronic stopping powers at energies above 100 MeV/amu which no Ziegler's formalism is valid are calculated using the Bethe-Bloch formula:

$$S = - \frac{4\pi e^4 N_A Z_1^2 Z_2}{m v^2 M_2} \left[\ln \frac{2mv^2}{I(1 - \beta^2)} - \beta^2 - \delta/2 - C/Z_2 \right], \tag{1.15}$$

where e and m are the charge and mass of an electron. v denotes the velocity of electrons, N_A the Avogadro's constant and C a term for the shell effect. I is the mean excitation potential[8] of orbital electrons in the target and δ a term for the density effect correction[8]. In OSCAR, the magnitude of the stopping powers at these energies is normalized by Ziegler's value at the energy of 100 MeV/amu.

1.5 Nuclear Stopping Power[3]

The nuclear stopping power at the projectile energy E is calculated using the Ziegler's formula:

$$S_n(E) = \frac{8.462 \cdot 10^{-15} Z_1 Z_2 M_1 S_n(\varepsilon)}{(A_1 + A_2)(Z_1^{0.23} + Z_2^{0.23})} 0.6022/M_2 \tag{1.16}$$

with

$$\varepsilon = \frac{32.53 A_2 E}{Z_1 Z_2 (A_1 + A_2)(Z_1^{0.23} + Z_2^{0.23})} \tag{1.17}$$

and

$$S_n(\varepsilon) = \frac{\ln(1 + 1.1383\varepsilon)}{2(\varepsilon + 0.01321\varepsilon^{0.21226} + 0.19593\varepsilon^{0.5})} \quad \text{for } \varepsilon \leqq 30, \tag{1.18}$$

$$S_n(\varepsilon) = \ln(\varepsilon)/2\varepsilon \quad \text{for } \varepsilon > 30, \tag{1.19}$$

where ε is the reduced energy of the projectile.

1.6 Stopping power of compound targets

The stopping power S_{comp} of compound targets is evaluated using Bragg's rule as follows;

$$S_{comp} = \Sigma_i N_i M_i S_i / M, \tag{1.20}$$

where M is the molecular weight of the compound target. M_i and N_i are the atomic weight and composition ratio of the i-th element in the compound target, respectively.

Appendix 2

Calculation of Projected Ranges

The projected range R_p is evaluated using Biersack's formula[3,5]. If the total stopping power and nuclear stopping power are available, the projected range for an element is expressed as

$$\left(S_t - \frac{\mu Q_n}{2E}\right)\frac{dR_p}{dE} = 1 - \left(\frac{\mu S_n}{2E} + \frac{\mu Q_n}{4E^2}\right) R_p \qquad (2.1)$$

with

$$\mu = A_2/A_1 .$$

Here, Q_n is the straggling of nuclear energy loss:

$$Q_n = \gamma W_n(\varepsilon) \qquad (2.2)$$

with

$$W_n = \frac{1}{4 + 0.197\varepsilon^{-1.6991} + 6.584\varepsilon^{-1.0494}} \qquad (2.3)$$

and

$$\gamma = 4A_1A_2/(A_1 + A_2)^2 . \qquad (2.4)$$

In OSCAR, the differential equation (2.1) is integrated using the Gauss-Legendre method to evaluate projected ranges. To obtain the projected ranges in compound targets, the following terms have to be converted for μS_n and μQ_n in Eq.(2.1):

$$\begin{cases} \langle \mu S_n \rangle = \sum_i \mu_i S_{ni} , & (2.5) \\ \langle \mu Q_n \rangle = \sum_i \mu_i Q_{ni} , & (2.6) \end{cases}$$

where μ_i, S_{ni} and Q_{ni} are the reduced mass, nuclear stopping power and straggling of the nuclear energy loss of the i-th element in the compound target, respectively.

Appendix 3
An Empirical Rule on the Excitation Functions

Let us pick up the position and height of the maximum for expressing the characteristics of the excitation function. Here, we particularly concern the systematics found for these quantities in the cases of the (q,xn)-type reactions, where q stands for incident charged particles including heavy ions. The resulting systematics would be able to extend, however, to the reactions involving charged particle emission if there were a sufficient number of data available for charged-particle-emitting reactions. The data used for deducing the systematics were mostly those compiled by Munzel et al.[36]

3.1 Position of the maximum

The reaction Q-value with sign reversed, -Q(q,xn), that roughly corresponds to the reaction threshold E_{th} as stated by Munzel et al. is a factor of shifting the peak of excitation function toward the high energy side. On the other hand, the descent of the excitation function is expected to begin as the rise of the excitation curve for the next neutron (or proton) emission. That is, the amount of the energy required for succeeding neutron or proton emission becomes another factor to determine the peak position. In the speculation, the controlling factor should be the smaller of the separation energies for the emitted neutron or proton. Here, the effect of the Coulomb barrier must be taken into account besides the separation energy for the latter.

Furthermore, the effect of the Coulomb suppression should be also considered. The cross section (thick and dotted lines in Fig.A-1) for the first step of the complete or incomplete fusion reaction is assumed to rise at the reaction threshold E_{th}, rapidly increase to the maximum height, and then remain constant thereafter. Excitation functions are approximated to be of similar features among various combinations of targets and projectiles. Only the differences are found in the E_{th} value and the height of the plateau. These assumptions are reasonable considering the results of the optical model calculation[37,38].

If the Coulomb barrier against the projectile is higher than the nominal reaction threshold obtained above, formation of the excited nucleus is suppressed. This effect may be expressed as the shift of the formation excitation curve (thick line in Fig.A-1) toward the high energy side as presented with a dashed line[39]. This effect of the excitation function results in the changes of the position and height of the maximum, from point p to p' in Fig.A-1, for the (q,n) reaction. Similar effects are observed even for (q,xn) reactions in the case of heavy nuclei.

In the case where outgoing particles possess the charge the energy required to surmount the Coulomb barrier will also appears in the equation giving the maximum position.

Finally, the kinetic energy of the emitted particles needs to be considered if the excitation energy corresponding to the maximum exceeds the minimum energy required for inducing the reaction. According to the evaporation model[40], the kinetic energy is approximated with twice the nuclear temperature T defined by[41]

$$\frac{1}{T} = \frac{d \ln\rho(E)}{dE} \qquad (3.1)$$

where $\rho(E)$ is the nuclear level density. If we neglect the difference between the nuclear and thermodynamic temperature, the temperature is calculated with the level density parameter a and residual energy U as

$$T = (U/a)^{1/2}. \qquad (3.2)$$

For the values of the level density parameters, the set given by one of the authors[4] was adopted because it reproduces well the neutron resonance data. Slightly better results were obtained for near magic nuclei with the set of a values compared to those with other sets, though no significant difference were observed in the off-shell region.

The simplest equation for the peak position, E_{max}, that satisfies the above consideration is expressed as

$$E_{max}(q,xn) = S[-Q(q,xn) + \min\{B_n(x+1),(B_p(x+1) + c_1E_c^{(p)})\}] + c_2S(\Delta E_c^{(q)}) + 2\sum_{i=1}^{x} T_i \qquad (3.3)$$

where min{A,B} implies the smaller of A and B, and $B_n(x+1)$ and $B_p(x+1)$ denote separation energies of neutron and proton, respectively, for the residual nucleus after x neutrons have been emitted. S(z) is a step function defined by

$$S(z) = \begin{cases} z & \text{for } z > 0, \\ 0 & \text{for } z \leqq 0. \end{cases} \qquad (3.4)$$

The first term, in the right hand side of Eq.(3.3) is considered to be the threshold for the successive particle emission. Here, $E_c^{(p)}$ represents the Coulomb barrier felt by the emitted proton, and the qauntity, $\Delta E_c^{(q)}$, designates the measure of the Coulomb suppression as defined by

$$\Delta E_c^{(q)} = E_c^{(q)} + Q(q,xn) - E_c^0 \ ; \quad E_c^0 = (Z_q + 4.5)\ \text{MeV} \qquad (3.5)$$

with the Coulomb barrier $E_c^{(q)}$ against the projectile q and the charge Z_q of q. The constants, c_1 and c_2, are adjustable parameters to be determined so as to reproduce the observed cross section data best.

3.2 Height of the maximum

The height of the plateau of the excitation function for the formation of the first step of the reaction depends upon the reaction mechanism. Here, we shall divide it into the following two categories; namely, reactions taking place in the nuclear core and those occurring at the edge. Complete and incomplete fusion (and knock-out reaction at high energies) be included in the former, while the latter covers inelastic scattering, nucleon transfer, charge exchange reaction, etc. We shall call the former the core reaction and the latter the peripheral reaction.

The height of the plateau of the excitation function for the formation of the excited states in the first step is expected to relate with the geometric cross section. In the step of the decay of the once-formed excited nucleus, the effect of the Coulomb barrier against the projectile must be considered as in the case of the position of the maximum.

Kinetic energies brought out by the emitted neutrons distribute within an energy range allowed from the energetics. It follows that the larger the available energy is, the broader the width of the excitation curve becomes ,as shown in solid curves in Fig.A-1. Increasing overlap with the neighboring excitation curves as the width increases lowers the height of the maximum. This effect is expressed as a monotonously decreasing function of a surplus energy:

$$\Delta E_{cm} = E_{cm} - E_0 = E_{max} - S[-Q(q,xn)] - E_0 \qquad (3.6)$$

with a critical energy:

$$E_0 = S[E_c^{(q)} - S\{-Q(q,xn)\}] + 7.0\ \text{MeV}. \qquad (3.7)$$

Difference in the difficulty of neutron emission between the successive steps affects their relative heights in the case of (q,xn) reactions. The effect depends on the degree of the neutron defficiency in the residual nucleus. A measure for such an effect would be given by difference in the mass excess between the primary excited and residual nuclei, and also the length of the evaporation chain. Competition among various decay modes affects the probability of the relevant decay mode. Generally speaking, however, the neutron width is predominant over charged particle widths except for the fission width of heavy elements as long as we concern light-ion induced reactions.

For high incident energies, one must consider the contribution of the non-compound type of reactions such as precompound decay or knock-out reaction. The effect of mixing of such non-equilibrium processes is assumed to appear only in the excitation energy left in the residual nucleus. That is, the nominal excitation energy be substituted with the effective excess energy E_{eff}. This substitution changes the maximum cross section σ_{max}. E_{eff} was found to be given by E_{cm} multiplied by a reducing factor α , which gradually decreases its value from unity as ΔE_{cm} increases beyond 2.5 MeV.

Summarizing the above well-founded conjectures, we obtained for the cross section for the core reaction at E_{max}:

$$\sigma_c(q,xn) = \pi r_0^2 A_2^{2/3} \prod_{i=1}^{x} P_{n,i} \exp\{-\lambda_1 S(\Delta E_c^{(q)}) - \lambda_2 S(\alpha E_{cm} - E_0) - \lambda_3 S(\Delta_n - \Delta_0)\}, \quad (3.8)$$

where $P_{n,i}$ gives the probability for the i-th neutron emission against the competing fission:

$$P_{n,i} = (1 + \Gamma_{f,i}/\Gamma_{n,i})^{-1} \quad (3.9)$$

with the partial level widths for neutron $\Gamma_{n,i}$ and fission $\Gamma_{f,i}$ of the i-th residual nucleus. Δ_n represents a measure of the hindrance against the cascade neutron emission:

$$\Delta_n = \{M(A_R) - M(A_0)\}S(A_0 - A_R) + \{M(A_I) - M(A_0)\}S(A_0 - A_I), \quad (3,10)$$

where A_0 is the nuclear mass number corresponding to the minimum mass excess in the neutron cascade chain and the suffixes I and R stand for initial and the residual nuclei, respectively, in the cascade chain. $r_0A_2^{1/3}$ is the radius of the target nucleus and λ_i (i=1 to 3) and Δ_0 are adjustable parameters.

For the peripheral reaction, the situation is considered more or less similar to the case of the core reaction, and so we took into account the contribution of the peripheral reaction merely by substituting the geometrical cross section $\pi r_0^2A_2^{2/3}$ in Eq.(3.8) by $\pi (r_0A_2^{1/3} + ƛ)^2$ at least for the (q,xn) reactions with projectiles not-heavier than 2; namely,

$$\sigma_{max}(q,xn) = \pi (r_0A_2^{1/3} + ƛ)^2 \prod_{i=1}^{x} P_{n,i} \cdot \exp(-\lambda_1 S(\Delta E_c^{(q)}) - \lambda_2 S(\alpha E_{cm} - E_0) - \lambda_3 S(\Delta_n - \Delta_0)), \qquad (3.11)$$

where ƛ is the reduced de Broglie wavelength.

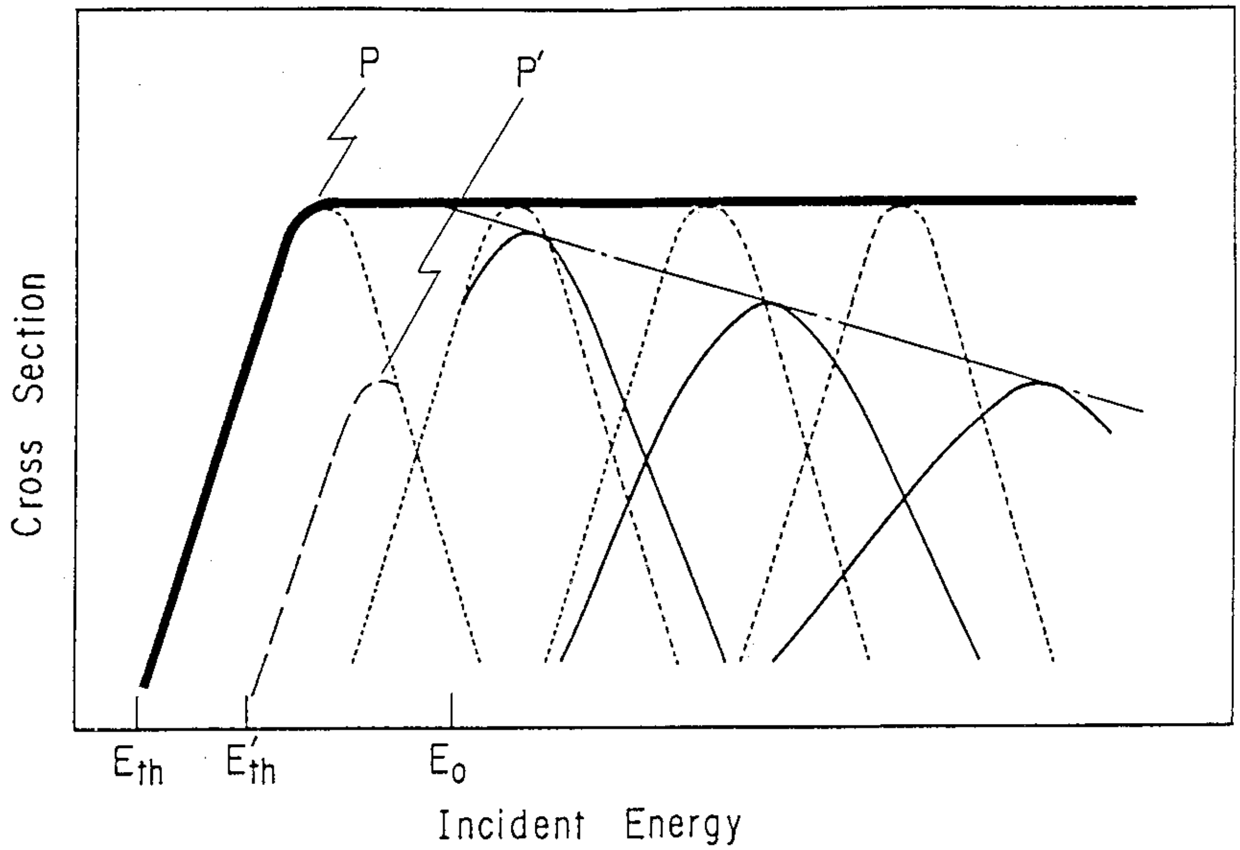

Fig. A-1 Schematic diagram of the excitation functions for fusion reactions and (q,xn)-type reactions. For details of the lines and symbols in the figure, the text should be referred to.