

Lawrence Berkeley National Laboratory

Recent Work

Title

PROGRAM BRAGG A FORTRAN-IV PROGRAM FOR CALCULATING BRAGG CURVES AND FLUX DISTRIBUTIONS

Permalink

<https://escholarship.org/uc/item/8s6804cp>

Author

Litton, Gerald M.

Publication Date

1967-02-24

University of California
Ernest O. Lawrence
Radiation Laboratory

PROGRAM BRAGG
A FORTRAN-IV PROGRAM FOR CALCULATING
BRAGG CURVES AND FLUX DISTRIBUTIONS

TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 5545*

Berkeley, California

34

UCRL-17391
C.2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Research and Development

UCRL-17391
UC-34 Physics
TID-4500 (49th Ed.)

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

PROGRAM BRAGG
A FORTRAN-IV PROGRAM FOR CALCULATING
BRAGG CURVES AND FLUX DISTRIBUTIONS

Gerald M. Litton^k

February 24, 1967

Printed in the United States of America
Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U.S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.65

PROGRAM BRAGG
A FORTRAN-IV PROGRAM FOR CALCULATING
BRAGG CURVES AND FLUX DISTRIBUTIONS

Contents

I.	General Description	1
II.	Mathematical Model	2
	A. Particle Energy Spectrum	2
	B. Number Density	4
	C. Dose	4
	D. Cross Sections	4
	E. Ionization-Energy Loss	5
	F. Straggling Parameter	5
	G. Multiple-Scattering Corrections	6
III.	Input Format	6
	A. Random Input System	6
	B. Notes on Control Card Use	9
IV.	Output Format	10
	A. Standard Output	10
	B. Optional Output	10
V.	Restrictions	12
	A. Mesh Size	12
	B. Initial Energy	12
	C. Target Components	12
	D. Input-Data Points	12
	E. Title Card	12
Appendixes		
	A. Numerical Procedures	13
	B. Notes on Compatibility	15
	C. Sample Problem	16
	D. Fortran Listing	24
References	67

PROGRAM BRAGG
A FORTRAN-IV PROGRAM FOR CALCULATING
BRAGG CURVES AND FLUX DISTRIBUTIONS

Gerald M. Litton

Lawrence Radiation Laboratory
University of California
Berkeley, California

February 24, 1967

I. GENERAL DESCRIPTION

Program BRAGG calculates Bragg curves and number-distance curves for a beam of ions of arbitrary atomic number, atomic weight, and energy, incident on an absorber. This absorber is assumed to be homogeneous, but may consist of an arbitrary number of components, each specified by an atomic number, atomic weight, and atomic density. The geometry considered is that of a broad, well-collimated beam incident on a slab whose transverse dimensions are large compared to the distance travelled by the ions in the absorber.

The calculation takes into account the processes of ionization energy loss, energy straggling, and nuclear attenuation; but energy deposition from secondary particles is neglected. The ionization energy loss and nuclear attenuation processes are calculated by means of distinct subroutines, which are intended for use either with protons or with ionized nuclei of heavy atoms. This flexibility has been deliberately incorporated, so that the user may easily employ his own routines for the calculation of these processes for any desired ion.

Corrections for multiple scattering have been included. The calculation of these corrections also produces estimates of range shortening and beam spreading due to the scattering process. These estimates are included in the program output.

Various options for data output are available. Bragg and number-distance curves may be printed in digital form, as on-line graphs, or as regular Cal-Comp plots. The Bragg curves may be normalized to an arbitrary quantity, either at the origin or at the Bragg peak. Similarly, the number-distance curve may be arbitrarily normalized at the origin.

For graphic display purposes, an option permits shifting the calculated Bragg curve so that the Bragg peak is set at a particular depth of penetration.

The program also calculates the particle energy spectrum at the Bragg peak. This may be printed out either in digital form or as a Cal-Comp plot.

Other options are available. Some of these pertain to control of the numerical procedure employed in the calculations, although the standard options that the program uses have been carefully chosen to yield the best results for most cases. An option is available that allows the user to choose an arbitrary value for the multiplication factor used in the calculation of the straggling standard deviation. The standard option is the theoretical value. Still another option pertains to the value of the nuclear-attenuation cross-section parameter. The standard option chosen is one that has been found to give reasonable agreement with experimental data.

For comparison purposes, input data may be supplied to the program. This data is then plotted along with any Cal-Comp figures output by the program.

Decks for Program BRAGG may be obtained from the Computer Center Library, Department of Mathematics and Computing, Lawrence Radiation Laboratory, Berkeley, California.

II. MATHEMATICAL MODEL

A detailed derivation and discussion of the equations upon which Program BRAGG is based is contained in UCRL-17392.¹ The purpose of this section is to outline briefly the basic mathematical expressions evaluated by BRAGG. All terms used are defined in Table I.

A. Particle Energy Spectrum

The spectrum at a given distance S is written as

$$M(E, S)dE = \frac{1}{\sqrt{\pi}} \cdot N_0(E_0) \cdot \exp \left\{ -A_p \int_E^{E_0} [\Sigma(E')/f(E')] dE' \right\} \cdot \exp[-U^2] \cdot [dU/dE] dE, \quad (1)$$

which is defined as the number of particles at S having energies within an interval dE about E . The function U is defined as

$$U = [S - \bar{S}(E)] / \alpha(E, E_0), \quad (2)$$

and

$$\bar{S}(E) = A_p \int_E^{E_0} [1/f(E')] dE', \quad (2a)$$

where $\bar{S}(E)$ is the mean distance travelled by particles slowing down from energy E_0 to energy E .

Table I. Nomenclature

A_i	Atomic weight of the i th species of the target
A_p	Atomic weight of beam ions
CRIT1	Constant appearing in the equation describing validity of the delta-function approximation
e	Electron charge in $(\text{cm-MeV})^{1/2}$
E	Energy of beam ions in MeV per nucleon
E_0	Initial energy of beam ions
$f(E)$	Specific ionization energy loss of ions of energy E , in $\text{MeV}/(\text{g}/\text{cm}^2)$
FR	Step-size criterion parameter, used in numerical integration scheme
IADJ	Input parameter used in calculation of $f(E)$
$D(S)$	Total energy deposition rate per unit distance of travel at position S , $\text{MeV}/(\text{g}/\text{cm}^2)/\text{sec}$
M_0C^2	Nucleon rest mass ≈ 938 MeV
$M(E, S)dE$	Number of ions per second with energies lying within an interval dE about energy E , at S
n	Number of electrons per cm^3 in the target
$N(s)$	Beam ion total-number flux at position S , in $\text{particles}/\text{cm}^2\text{-sec}$
$N_0(E_0)$	Initial number flux at target surface, in $\text{particles}/\text{cm}^2\text{-sec}$
N_i	Atom density of the i th species of the target, in $\text{No.}/\text{cm}^3$
NT	Number of species in target
r_0	Total reaction-cross-section parameter
S_0	Parameter connected with range straggling calculation
S	Distance of travel in the target, in g/cm^2
$\bar{S}(E)$	Mean distance travelled by ions slowing down from energy E_0 to energy E
Z_i	Atomic number of i th species of the target
Z_p	Atomic number of beam ions
ϵ	Total energy in the center-of-mass system
ρ	Target density, in g/cm^3
$\sigma(E)$	Standard deviation of ions slowing down to zero from energy E
$\sigma(E, E_0)$	Standard deviation of ions slowing down from energy E_0 to energy E
$\eta_i(E)$	Microscopic total-reaction cross section for beam ions with energy E with the i th target species
$\lambda(E)$	Wavelength of beam ions with energy E
$\Sigma(E)$	Macroscopic total-reaction cross section for beam ions with energy E with the target.
$\alpha(E)$	Straggling parameter of ions slowing down to zero from energy E
$\alpha(E, E_0)$	Straggling parameter of ions slowing down to energy E from energy E_0

B. Number Density

The particle number density, also denoted as the number flux, or simply flux, is given at a particular distance S by

$$N(S) = \int_{\text{all } E} M(E, S) dE, \quad (3)$$

where $M(E, S)$ is given by Eq. (1). The curve describing the variation of $N(S)$ with S is called the number-distance curve.

C. Dose

The relative dose at a distance S is given by

$$D(S) = \int_{\text{all } E} M(E, S) \cdot f(E) dE. \quad (4)$$

D. Cross Sections

The total microscopic reaction cross section for the i th component of the target at a particular energy E is calculated from an expression developed by Evans² and is given as

$$\eta_i(E) = \pi \left[r_0 \times 10^{-13} (A_p^{1/3} + A_i^{1/3}) + \lambda \right]^2 \left[1 - \frac{Z_i Z_p e^2}{\epsilon [r_0 \times 10^{-13} (A_p^{1/3} + A_i^{1/3}) + \lambda]} \right], \quad (5)$$

where the particle wavelength is

$$\lambda = (\hbar c / A_p)^{1/2} [2E(\text{MoC}^2) + E^2]^{1/2}, \quad (6)$$

and the CM energy is

$$\epsilon = \frac{A_i \cdot A_p}{A_p + A_i} E. \quad (7)$$

The term r_0 is an input parameter chosen so as to best fit the experimental data. Work has shown that a value of 1.06 for r_0 gives best agreement with many experimental results. This value is used by the program, unless the user specifies otherwise.

The total macroscopic cross section is given by the expression

$$\Sigma(E) = \sum_i \eta_i(E) N_i. \quad (8)$$

E. Ionization Energy Loss

The function $f(E)$ represents the specific energy loss of the ions due to ionization interactions with the atoms of the absorber. The calculation of this function is incorporated into a series of subroutines, and is based entirely on the work of Steward and Wallace.³

One important input parameter required for the calculation of $f(E)$ is IADJ, which is related to the mean excitation energy for a particular absorber. The significance of this quantity is discussed by Barkas and Berger,⁴ and a tabulation of values for all elements is given by Turner.⁵

F. Straggling

The variance in the distance of travel of ions slowing down from energy E_0 to energy E is given as

$$\sigma^2(E, E_0) = \sigma^2(E_0) - \sigma^2(E), \quad (9)$$

where $\sigma^2(E)$ is the variance for ions slowing down to zero from E . It is calculated by the following expression, a modification of that derived by Sternheimer.⁶

$$\sigma^2(E_0) = 4\pi Z_p^2 e^4 n \int_0^{E_0} \frac{1+H(E)}{H(E)} \frac{dE}{[f(E)]}, \quad (10)$$

where

$$H(E) = \left(\frac{M_0 C^2}{E + M_0 C^2} \right)^2. \quad (10a)$$

The straggling parameter $\alpha(E, E_0)$ is given by

$$\alpha(E, E_0) = S_0 \cdot \sigma(E, E_0). \quad (11)$$

The theoretical value of S_0 is equal to $\sqrt{2}$. However, the user may at his option choose a different value.

G. Multiple-Scattering Corrections

Because of small-angle multiple-scattering, slight corrections must be applied to the calculated dose and flux distributions. (Although the magnitude of these corrections is small, the expressions for them are long and tedious and will not be reproduced here. Reference is made instead to UCRL-17392.) One result of these calculations is an estimate of range shortening and beam spreading due to the scattering.

III. INPUT FORMAT

In the deck of input cards, the first card specifies the number of individual problems to be run, in (I10) format. Following this card is a separate data deck for each problem to be run. Each deck is arranged in the Random Input System, making input extremely easy and efficient.

A. Random Input System

The basic advantage of this system is that within a given data deck, the input cards may be arranged in any desired order, and one must supply only those cards necessary to the particular problem being run.

The deck consists of control cards and data cards. Data cards are seldom used, being necessary only when space on the associated control card is insufficient for the data being supplied by that control card. The first field on a control card indicates to the program which control card is being examined. In some cases, this field by itself specifies a particular option to be followed by the program. In other cases, the remaining fields supply data to the program. In a few cases, a control card will indicate that a number of specific data cards immediately follow.

The format of all control cards is (A10, 3E10.0, 2A10). The first field contains an alphanumeric identifier, always left-justified. The remaining fields may or may not contain data, depending on the card. Table II gives a complete list of the control cards available as input to BRAGG. For several cards, the standard option is indicated in the table. This is the option chosen by the program in the absence of a control card specifying otherwise. In many cases, the standard option is the opposite of the control card specification and is not indicated in the table. For example, the PRINT DOSE control card specifies the printing of certain information. In the absence of this card, the information will not be printed.

A blank control card indicates the end of card input for that problem. Upon termination of a problem, the program reads in another data deck (the last card again being blank). The program terminates after the number of problems specified by the initial data card has been run.

Table II. Control Cards

Columns 1 through 10	Function
BEAM	(a) Z_p and A_p in fields 2 and 3. (b) Beam designation (alphanumeric identifier) in fields 5 and 6.
ENERGY	Beam energy (MeV/nucleon) in field 2.
TITLE	Read the 80-character title from the next card.
TARGET*	(a) NT, target specific gravity and value of IADJ in fields 2, 3, and 4. (b) Target designation (alphanumeric identifier) in fields 5 and 6. (c) Read (Z_J , N_I , A_J , $J = 1$, NT) from the next NT cards, in (3E10.0) format.
PRINT DOSE	Print the dose and particle-number density at all points calculated.
PRINT E	Print the energies at which computations are performed.
PRINT SPEC	Print the particle energy spectrum at the Bragg peak.
PRINT SIG	Print the particle survival fraction, straggle parameter, and mean energy at all points calculated.
LET NORM-P	Normalize the calculated dose distribution so that the dose at the Bragg peak is equal to the quantity in field 2. (Standard option: unnormalized.)**
LET NORM-I	Normalize the calculated dose distribution so that the initial dose is equal to the quantity in field 2. (Standard option: unnormalized.)**
FLUX NORM	Normalize the particle flux distribution so that the initial flux is equal to the quantity in field 2. (Standard option: normalize to 1.0.)**
X-ADJUST	Shift the calculated Bragg curve so that the peak occurs at the penetration distance value, in g/cm^2 , given in field 2.
PLOT DOSE	Produce a Cal-Comp graph of the Bragg curve.
PLOT FLUX	Produce a Cal-Comp graph of the number-distance curve.
DATA	(a) ND in field 2. (b) Read ND data points from the cards immediately following. The order of the input points is YDATA (I), XDATA (I), with one data point to a card in (2E10.0) format.
PLOT DATA	Plot the data points last read in with a DATA control card.***
SAME CURVE	Plot the curve for the current problem on the same figure as that of the preceding problem.***
PLOT SPEC	Produce a Cal-Comp graph of the spectrum at the Bragg peak.

Table II. (Continued)

Columns 1 through 10	Function
CRIT1	Set CRIT1 equal to the value in field 2. (Normal option: 0.01).
FR	Set FR equal to the value in field 2. (Normal option: 0.2).**
QUICKPLOTD	Produce an on-line graph of the Bragg curve.
QUICKPLOTN	Produce an on-line graph of the number-distance curve.
RZERO	Set r_0 equal to the value in field 2. (Normal option: 1.06).**
SIGMULT	Set S_0 equal to the value in field 2. (Normal option: $\sqrt{2}$).**
PRINT SCAT	Print intermediate information produced in the multiple-scattering calculations
CALL TABLE	Print the information on file TAPE5 in tabular form and request the file (See Section B-3).****

* See Section B-7.
 ** See Section B-1.
 *** See Section B-2.
 **** See Section B-3.

B. Notes on Control-Card Use

1. In certain cases, once a particular option has been chosen, it will remain in effect for all of the remaining problems in a set, or until another control card changes the option. The options for which this is true are indicated by a double asterisk in Table II. For example, insertion of the control card LET NORM-P, with a 1.0 punched in the second field, will cause the calculated Bragg curves for each of the remaining problems to be normalized to unity at the peak.

Control cards not asterisked must be inserted in the data deck of each problem for which that option is to be exercised.

2. In using options for producing Cal-Comp graphs, the following points should be remembered. A PLOT DATA control card will cause the program to plot the data points with each figure produced during the execution of a given problem. Therefore, it would normally be used when only one graph is to be plotted during a given problem. Similarly, the SAME CURVE control card prevents frame-advancing and axis-labelling during a given problem. It is normally used to plot several Bragg curves or number-distance curves from successive problems on the same figure. Therefore, if either a PLOT DATA or SAME CURVE card is present in the data deck for a given problem, not more than one of the control cards PLOT SPEC, PLOT FLUX, or PLOT DOSE should be in that deck.

3. During execution, the standard printout consists of several key results, described in Section IV-A. These quantities are also written on the file TAPE5 at the completion of each problem. Insertion of a CALL TABLE control card during a particular problem causes the following sequence: (1) After successful completion of the problem, TAPE5 is rewound; (2) All results on TAPE5 are printed on the standard output file in convenient tabular form; (3) TAPE5 is rewound.

4. Regardless of the context, the quantities appearing in fields 2, 3, and 4 of any control card must have a decimal point or be right-justified within the field.

5. Data points supplied by the DATA control card may be either for Bragg or number-distance curves or for the Bragg-peak spectrum. Once read in, a set of data points remains in storage until a new set is read in.

6. The on-line plotting option, via the control cards QUICKPLOTN and QUICKPLOTD, can be used only if one or more data points have been supplied by a DATA card.

7. With the TARGET control card, NT is the number of components of the target; it is also equal to the number of data cards immediately following the TARGET card. Note that N_j is equal to the atom density times the factor 10^{-22} .

IV. OUTPUT FORMAT

A. Standard Output

Various output options are available to the user by means of control cards. In all cases a certain amount of standard output is produced. This consists of a synopsis of the input data and a summary of key results. The first section includes the following:

1. Beam atomic number, atomic weight, and initial energy;
2. Target specific gravity and value of IADJ;
3. Atomic number, atomic weight, and atom density of each component of the target;
4. Values to be used by program for CRIT1, FR, r_0 , and S_0 . In addition, messages are printed indicating the modes to be used for flux and dose normalization and for axis shifting.

The second section of standard output contains the following:

1. The peak-to-initial-dose ratio;
2. The depth of penetration at the Bragg peak;
3. The average energy at the Bragg peak;
4. The full width at half-maximum of the Bragg peak;
5. The mean range, defined as the penetration distance at which the dose has fallen to one-half that at the peak;
6. The percentage-detour factor, which is the percentage difference between the mean distance of travel and the corresponding penetration distance calculated at that point at which the dose is equal to ten percent of the peak dose;
7. The mean beam deflection, equal to the mean distance of travel in a direction perpendicular to the initial direction of travel of the beam. It is calculated at the same position as is the percentage-detour factor.

All energies are measured in units of MeV/nucleon, and all distances in units of g/cm^2 .

B. Optional Output

The PRINTE card causes the program to print a list of the particle energies at which calculations are performed. The relationship between a given energy and the corresponding mean distance of travel is given by Eq. (2a).

The PRINT SIG card causes the program to list, at each particle energy at which calculations are performed, the following quantities:

1. The energy;
2. The survival fraction, equal to the fraction of particles which have survived to that energy without undergoing a nuclear interaction;
3. The corresponding straggle parameter, given by Eq. (11);
4. The corresponding penetration distance into the slab, equal to that

distance given by Eq. (2a) modified slightly to take into account the multiple-scattering correction.

The PRINT DOSE control card causes the following quantities to be listed:

1. The penetration distance (same as 4 above);
2. The normalized or unnormalized flux, given by Eq. (3);
3. The normalized or unnormalized dose, given by Eq. (4);
4. A calculation-mode indicator. If the indicator is "MON", at that point calculations were made using the delta-function approximation (see APPENDIX A). If the indicator is "SUM", then the dose and flux were calculated by standard numerical integration. Finally, if the indicator is "SUMI", the depth of penetration was greater than $\bar{S}(0)$, given by Eq. (2a).

The PRINT SCAT control card causes the printing of miscellaneous quantities associated with the calculation of the multiple-scattering corrections, including:

1. The energy;
2. The actual mean distance of travel corresponding to that energy given by Eq. (2a);
3. The corresponding penetration distance;
4. The mean angle of deflection made by the particles with respect to the initial direction of travel;
5. The mean beam deflection, a quantity expressing the mean distance travelled by the particles in a direction perpendicular to the initial direction of travel;
6. The quantity THETAS, equal to the mean angle of deflection of the particles per unit length of travel. Its significance is discussed in UCRL-17392.

The PRINT SPEC card produces a printout of the energy spectrum at the Bragg peak, calculated by use of Eq. (1). This spectrum is automatically normalized to unity at the peak. It should be mentioned that the average energy at the peak is calculated by using this spectrum as a weighting function.

Use of the QUICKPLOTD and (or) QUICKPLOTN control cards will produce a plot of the dose and (or) number-distance curve on the standard output unit.

Several options may be exercised in the printing of Cal-Comp plots. First, regular plots may be produced for any or all of the three calculated curves (Bragg, number-distance, and peak spectrum) within a given problem by use of one or more of the PLOT DOSE, PLOT FLUX, and PLOT SPEC control cards. In all cases, the axes are automatically labelled and numbered. Furthermore, a title is affixed to each figure produced. This is supplied by the TITLE control card. If a title is to be printed on a graph, it must not exceed 43 BCD characters. Any excess above this number will be lost. All plotted figures are sized to the standard $8\frac{1}{2}$ by 11-in. sheet.

The DATA and PLOT DATA control cards may be used to plot experimental data along with either a Bragg, number-distance, or peak-spectrum curve. The SAME CURVE control card may be used to overlay curves from different problems on the same figure, for comparison and display purposes. (See Section III-C-2.)

V. RESTRICTIONS

A. Mesh Size

The maximum allowable number of mesh points for a problem is 500. The total number of mesh points used depends on many variables, the chief ones being FR and CRIT1. The standard options used for these variables will normally keep the number of mesh points well below 500. If different values are used, the number of points can in some cases exceed 500. If this occurs, an error message is printed, and the program goes on to the next problem.

B. Initial Energy

The maximum allowable initial energy is 1000 MeV/nucleon. This restriction is imposed by the routines that calculate $f(E)$, and it can easily be modified.

C. Target Components

The maximum number of components of the target is set at 10.

D. Input-Data Points

The maximum number of data points that may be read in with a DATA control card is set at 300.

E. Title Card

The BCD characters on the card following the TITLE control card will be printed on any Cal-Comp plots produced. In this case, characters in excess of 43 will not be plotted. In all cases, the full 80-characters are printed along with the output.

APPENDIXES

A. Numerical Procedures

1. Delta-Function Approximation

We consider the evaluation of the expression given by Eq. (4), and the associated expressions in Eq. (1) and (2). For sufficiently small values of $\alpha(E, E_0)$, the term $(1/\sqrt{\pi}) \cdot \exp\{-U^2\} [dU/dE]$ behaves like a delta-function; and Eq. (4) reduces to

$$D(\bar{S}) = N_0(E_0) \exp \left\{ -A_p \int_E^{E_0} [\Sigma(E')/f(E')] dE' \right\} f(E) \quad (12)$$

where \bar{S} is given by Eq. (2a). We wish to learn when this approximation is valid. This may be deduced by the following argument. Consider the exponential term

$$T = \exp\{-U^2\}, \quad (13)$$

where U is given by Eq. (2). For a given value of S , T is the controlling factor in determining how rapidly the total integrand in Eq. (4) goes to zero. Thus, for $U \geq 3$, the contribution to the total integrand will be negligible. Therefore, if each and every other factor in the integrand remains relatively constant over the energy interval within which the integrand differs significantly from zero, then the approximation of (4) by (12) is valid.

We state this mathematically as follows. Let D be the range covered by the variable $\bar{S}(E)$ over which the term T is significantly greater than zero. We may write

$$D = M \cdot \alpha(E, E_0), \quad (14)$$

where M is some constant in the neighborhood of 2 to 3. We wish to calculate the change in energy, ΔE , corresponding to the distance D . From Eq. (2a), we find that for a change in $\bar{S}(E)$ equal to D , the corresponding change in energy is approximately

$$\Delta E \approx \frac{D}{A_p} \cdot f(E) = M \cdot \alpha(E, E_0) \cdot f(E) \cdot \frac{1}{A_p}. \quad (15)$$

We now require that the percentage change in each other factor in the integrand be less than some fraction h over the energy interval ΔE given by (15). The two functions to consider are:

$$G_1(E) = \exp - \int_E^{E_0} A_p \cdot [\Sigma(E')/f(E')] dE', \quad (16)$$

and

$$G_2(E) = f(E). \quad (16a)$$

For a given function $G_i(E)$, the percentage change over an increment ΔE is approximately

$$\frac{\Delta G_i}{G_i}(E) \approx \frac{dG_i(E)}{dE} \cdot \frac{\Delta E}{G_i(E)}. \quad (17)$$

Taking the derivatives of both functions in (16), using the approximation in (17) and the expression for ΔE in (15), and requiring that the percentage change of each function over ΔE be less than h , we obtain the following criteria:

$$\Sigma(E) \cdot \alpha(E, E_0) < \text{CRIT1} \quad (18)$$

and

$$\frac{dF(E)}{dE} \cdot \alpha(E, E_0) < A_p \cdot \text{CRIT1}, \quad (18a)$$

where

$$\text{CRIT1} = h/M. \quad (19)$$

If both of these requirements are satisfied for a reasonable value of h/M , then Eq. (4) may be replaced by the much simpler Eq. (12). Similarly, if Eq. (18) holds, then Eq. (3) may be replaced by the following:

$$N(S) = N_0(x) e^{-\int_E^{E_0} \frac{\Sigma(E')}{f(E')} dE'}. \quad (20)$$

Experiment has shown that a value of CRIT1 equal to 0.01 produces excellent results. For larger values, the delta-function approximation begins to break down.

2. Numerical Integration

For those points at which the delta-function approximation is invalid, the integrals in Eq. (3) and (4) are evaluated numerically, using the simple trapezoidal rule. In this case, the procedure is basically as follows:

1. Choose a set of energies $\{E_i\}$.
2. Calculate the set $\{\bar{S}_i\} = \{\bar{S}(E_i)\}$ for each energy by using Eq. (2a).
3. Calculate $\alpha(E, E_0)$ for each energy by using Eq. (11).
4. Evaluate the integral $\int_E^{E_0} A_p [\Sigma(E')/f(E')] dE'$ at each energy.

Finally, the numerical integration is performed for a set of values for the distance S . In fact, the evaluation is greatly simplified by choosing these values to coincide with the set $\{\bar{S}_i\}$.

It remains to choose the energy set $\{E_i\}$ at which the numerical calculations are to be performed. Since the term T given by (13) is the most rapidly varying in both (3) and (4), we impose the requirement that in traversing the energy interval ΔE , which is the interval over which the trapezoidal rule is applied at any given step, the change in the quantity U be less than or equal to some fraction FR , where FR is a small fraction of unity.

This ensures that the change in the exponential term T will likewise be small over the interval ΔE .

The change in U across ΔE is approximated by

$$\Delta U \cong \Delta \bar{S} / \alpha(E, E_0), \quad (21)$$

where $\Delta \bar{S}$ is the difference between two successive members in the set $\{\bar{S}_i\}$.

It is assumed that $\alpha(E, E_0)$ remains relatively constant over the interval. We require, then, that

$$\Delta S / \alpha(E, E_0) \leq FR. \quad (22)$$

From Eq. (2a), the relation between the change in distance $\Delta \bar{S}$ and the corresponding energy change ΔE is

$$\Delta E = \frac{1}{A_p} \cdot f(E) \cdot \Delta \bar{S}. \quad (23)$$

Substituting into (22), we obtain the restriction on ΔE :

$$\Delta E \leq \frac{1}{A_p} \cdot f(E) \cdot \alpha(E, E_0) \cdot FR. \quad (24)$$

Thus, for a given energy E_i , the next energy E_{i+1} at which the calculations are performed is given by (24) where the equality sign is chosen. Therefore we can write

$$E_{i+1} = E_i - \Delta E. \quad (25)$$

Experimentally, it is found that a value for FR of 0.2 is satisfactory.

B. Notes on Compatibility

Program BRAGG is written in Fortran-IV language for the Control Data Corporation 6600 computer system at the Lawrence Radiation Laboratory (LRL) in Berkeley, California. It can be used with a minimum of modification on practically any system that accepts Fortran-IV and that has adequate storage capacity. The chief alterations that might have to be made are outlined below.

1. Word Size

The CDC-6600 operates on a word size of 60 bits, or ten BCD characters. For machines using different word sizes, all instructions depending on the word size would have to be modified. These would be primarily the DATA statements appearing at the beginning of the main program;

some of the WRITE or PRINT statements (and their associated FORMAT statements) that appear in the main program and in the subroutines GMPRINT and TABLE; and the series of LOGICAL IF statements appearing in the main program after statement 501.

2. Graphing Routines

BRAGG contains the option of producing Cal-Comp drawn figures; the control statements for this process are contained in SUBROUTINE GMPRINT, and many of them refer to subroutines peculiar to LRL Berkeley. At other installations, these statements might have to be removed or replaced.

3. ENCODE and DECODE Statements

These statements occur in the subroutines FIXLBL, CENTER, and GMPRINT. The easiest method of eliminating these statements is by a set corresponding WRITE and READ statements to a scratch file.

4. CALL DATE Statement

This occurs in the beginning of the main program and in subroutine TABLE. DATE is an LRL routine which supplied the current date.

5. Input-Output Statements

The input and output statements may each take any of several forms; not all of these forms may be allowed on other systems.

C. Sample Problem

The input and output for a typical problem are given here. The case chosen is for 125-MeV protons in water. Only the standard printed output is selected, but Cal-Comp plots are shown for all three calculated curves.

Figure 1 shows the input cards for the problem. The three pages following Fig. 1 show the standard output. Figures 2, 3, and 4 show the Cal-Comp plots of the Bragg curve, the number-distance curve, and the spectrum at the Bragg peak.

04/27/67.

-----PROGRAM BRAGG-----

SAMPLE PROBLEM WITH PROGRAM BRAGG

-----INPUT DATA-----

BEAM PARTICLES	BEAM AT. NO.	BEAM AT. WT.	BEAM INITIAL ENERGY
PROTONS	1	1.00	125.00
CRIT1	FR	SIGMULT	RZERO
1.0000E-02	2.0000E-01	1.414	1.0600E+00

NO ADJUSTMENT OF THE ABSCISSAS HAS BEEN MADE

THE LET-DISTRIBUTION IS NORMALIZED TO 1.0000E+00 AT THE BRAGG PEAK

NO NORMALIZATION OF THE NUMBER-DENSITY DISTRIBUTION IS MADE

-----TARGET DATA-----

MATERIAL DESIGNATION SPECIFIC GRAVITY IADJ
WATER 1.000 65.10

NUMBER OF COMPONENTS IN TARGET MATERIAL..... 2

COMPONENT	ATOMIC NUMBER	ATOMIC WEIGHT	ATOM DENSITY (NO. PER CM**3)
1	8	16.000	3.3500E+22
2	1	1.000	6.6900E+22

04/27/67.

SUMMARY OF RESULTS

SAMPLE PROBLEM WITH PROGRAM BRAGG

(BRAGG PEAK/INITIAL) DOSE RATIO..... 6.5298

PENETRATION DEPTH AT BRAGG PEAK (G/CM**2)..... 11.1503

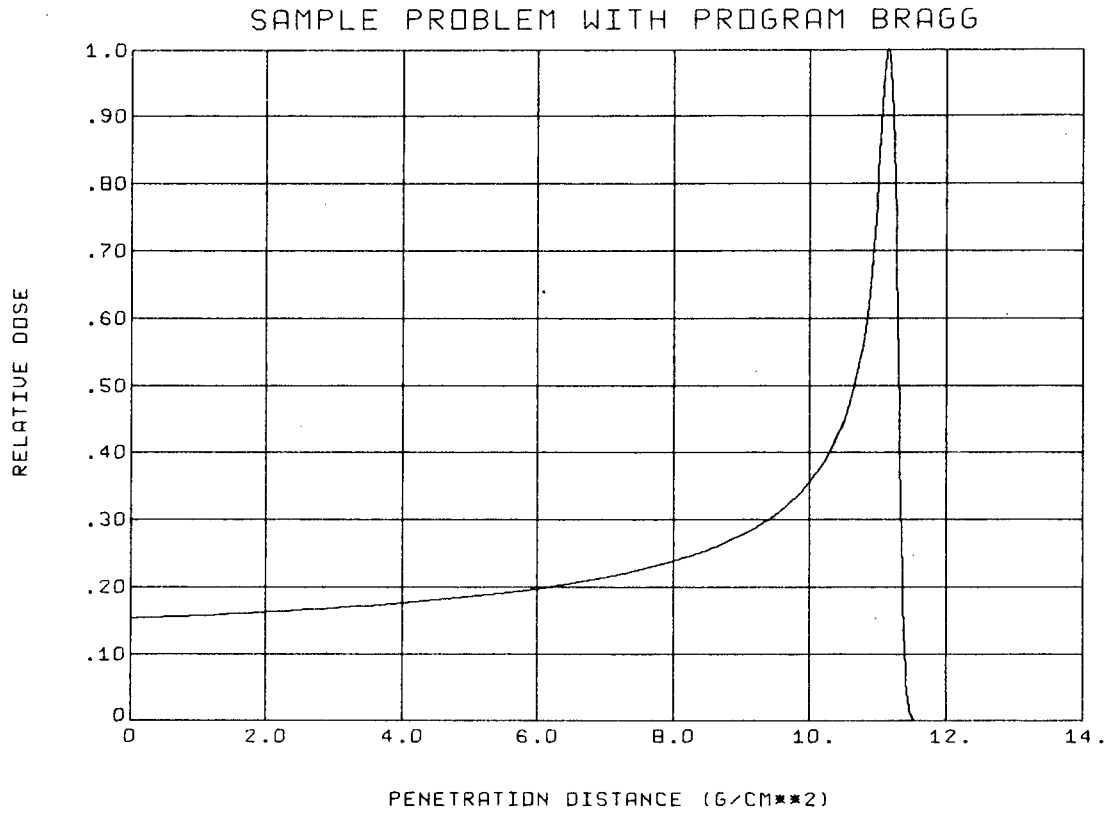
AVERAGE ENERGY AT BRAGG PEAK (MEV/NUCLEON)..... 10.1360

BRAGG PEAK FULL WIDTH AT HALF-MAXIMUM..... 6.476E-01

MEAN RANGE (G/CM**2)..... 11.3042

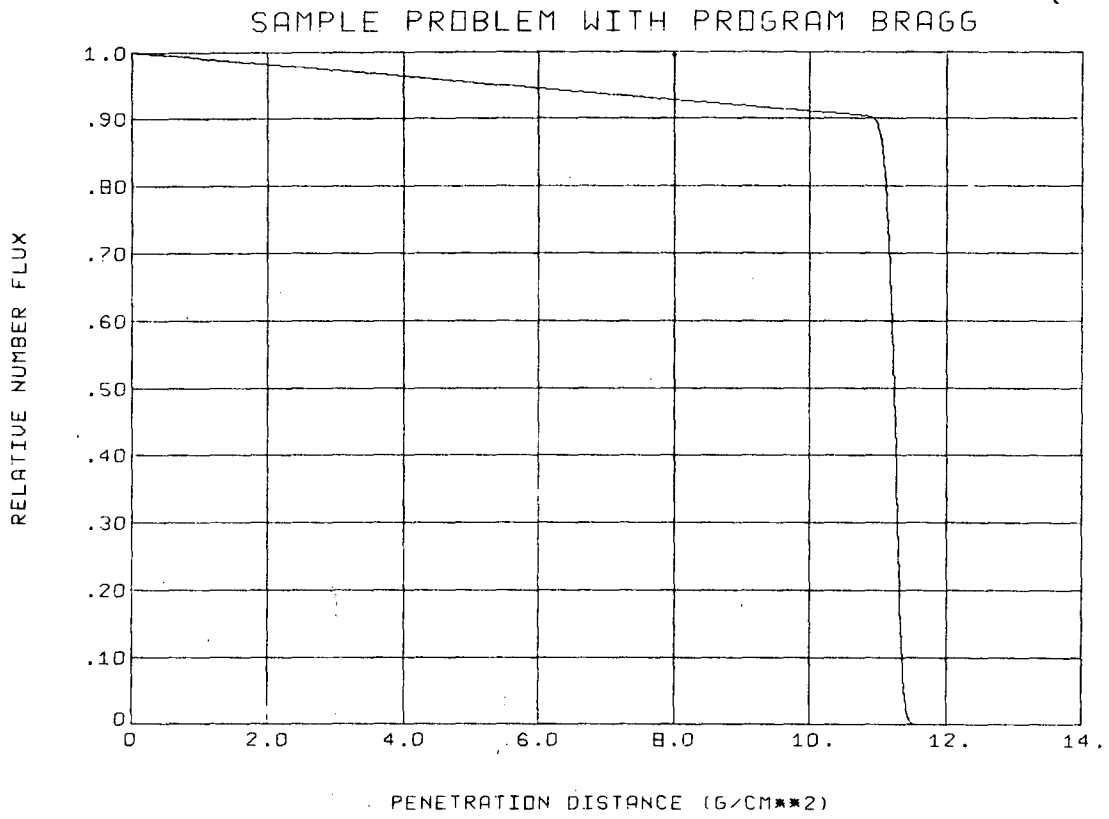
PERCENTAGE DETOUR FACTOR..... .6200

MEAN LATERAL DISPLACEMENT OF BEAM (G/CM**2)..... 5.041E-01



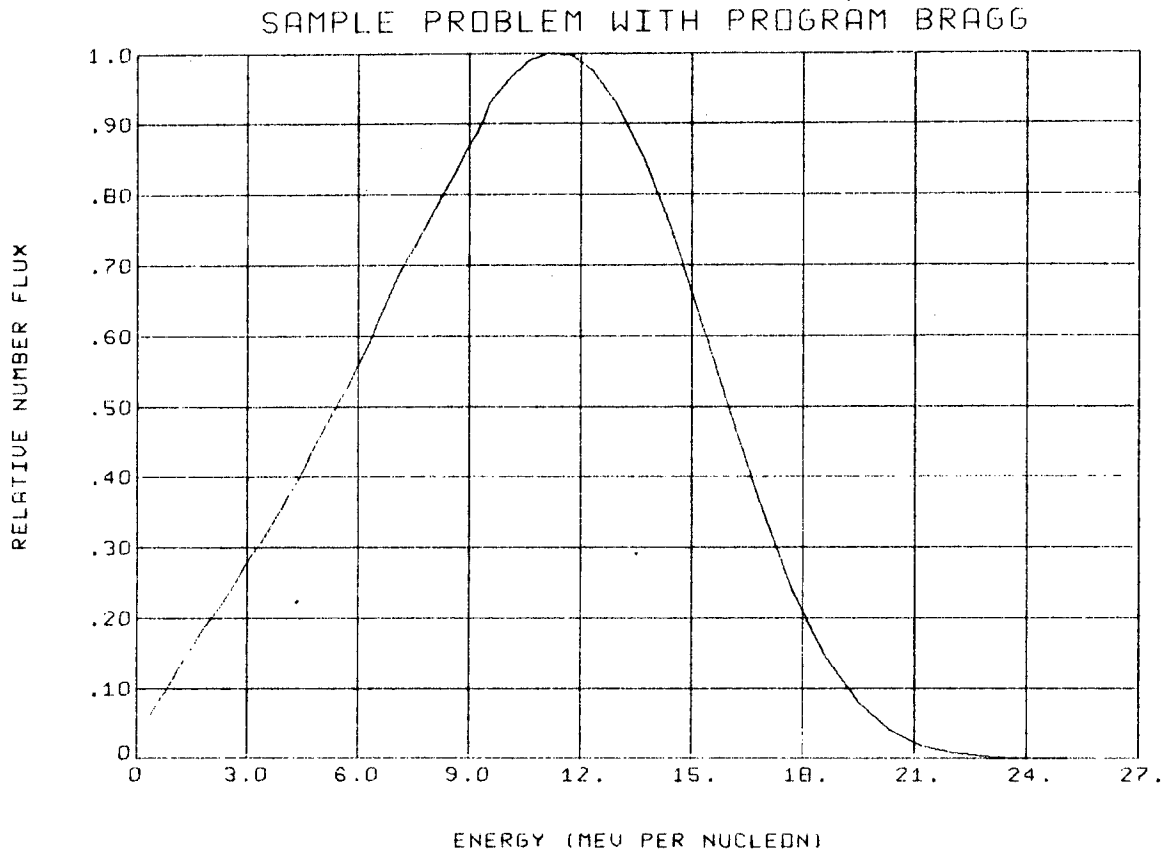
XBL 675-4001

Fig. 2. Cal-Comp plot of Bragg curve for sample problem.



XBL 675-4002

Fig. 3. Cal-Comp plot of number-distance curve for sample problem.



XBL 675-4003

Fig. 4. Cal-Comp plot of spectrum at the Bragg peak for sample problem.

D. Fortran Listing

This section contains the complete Fortran listing of Program BRAGG. All subroutines used are included, except for Cal-Comp plotting subroutines and system routines for input, output, and other standard functions:

```

PROGRAM BRAGG(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT,TAPE98,TAPE99,
2 TAPE5)
REAL M,INT,N,MAT,BEAM,LET,IADJ,NELECT
LOGICAL EPRINT,SGPRINT,DPRINT,SPPRINT,PRTABLE,PRSCAT,KPLOTN,
2 KPLOTD,FRAME,PLOTD,PLOTN,PLOTSP,PLOTP
DIMENSION MAT(2),BEAM(2),XNAME(15),FMT(2),TITLE(15)
DIMENSION GG(500),SAVE1(500),CROSS(500),U(500),DUDE(500)

COMMON ATEN(500),SBAR(500),E(500),SIGMA(500),IND(500),LET(500),
2 N(500),SPECT2(500),THETAS(500),THETA(500),XBAR(500),Y(500),
3 XDATA(300),YDATA(300),F(500)
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
COMMON/DATA/NDTAPT,PLOTP
COMMON /GMDATA2/TITLE,FRAME,INNP,KS1,KS2
COMMON/GMDATA1/IMAX,DIFF,I8,PD
COMMON/GDATA2/RHO,RZERO
EQUIVALENCE      (GG,SAVE1,THETA),(U,THETAS),(Y,CROSS,DUDE)
DATA

2COM1 /6HTARGET      /,COM2 /4HBEAM          /,COM3 /9HCRT1      /,
3COM4 /9HFR          /,COM5 /6HENERGY       /,COM6 /10HLET NORM-P/,
4COM7 /9HFLUX NORM  /,COM8 /8HX-ADJUST     /,COM9 /10HPRINT SIG /,
5COM10/10HPRINT DOSE/,COM11/10HPRINT SPEC/,COM12/10HPRINT E   /,
6COM13/10HQUICKPLOTD/,COM14/9HPLOT DOSE   /,COM15/9HPLOT FLUX /,
7COM16/10HSAME CURVE/,COM17/5HTITLE      /,COM18/10HPLOT SPEC /,
8COM19/10HQUICKPLOTN/,COM20/10HRZERO      /,COM21/10HCALL TABLE/,
9COM22/10HLET NORM-I/,COM23/10HPRINT SCAT/,COM24/10HPLOT DATA /,
1COM25/10HSIGMULT   /,COM26/10HDATA      /

DATA TITLE/15*10H
DATA JDEX1,JDEX2/10HMON      ,10HSUM
DATA JDEX3/10HSUMI
DATA (XNAME(I),I=1,15),XMASK/16*1H

M(U)=(0.56419)*EXP(-{U**2})
H(E)=(921.3/(921.3+E)**2)
G(E)=(1.3027E-25)*(Z**2/RHO)*NELECT*(1.0+H(E))/H(E)

CALL CCBGN
REWIND 5
ASSIGN 770 TO NNN1
ASSIGN 767 TO NNN2
LNORM=0
FR=0.2
CRIT1=0.01
CONST1=0.0
CONST2=0.0
CALL DATE(TTDATE)
SIGMULT=1.414
RZERO=1.06
READ(2,100)NNP
DO 1000 INNP=1,NNP
WRITE (3,114)
WRITE(3,110) TTDATE
XADJ=0.0
FRAME=.TRUE.
PLOTD=.FALSE.
PLOTN=.FALSE.
PLOTSP=.FALSE.

```

```
PLOTP=.FALSE.
KPLOTD=.FALSE.
KPLOTN=.FALSE.
PRTABLE=.FALSE.
PRSCAT=.FALSE.
DPRINT=.FALSE.
SGPRINT=.FALSE.
SPPRINT=.FALSE.
EPRINT=.FALSE.
501 READ (2,101) TEMP1,TEMP2,TEMP3,TEMP4,TEMP5,TEMP6,TEMP7,TEMP8
  IF(TEMP1.EQ.XMASK)GO TO 515
  IF(TEMP1.EQ.COM1)GO TO 502
  IF(TEMP1.EQ.COM2)GO TO 503
  IF(TEMP1.EQ.COM3)CRIT1=TEMP2
  IF(TEMP1.EQ.COM4)FR=TEMP2
  IF(TEMP1.EQ.COM5)GO TO 506
  IF(TEMP1.EQ.COM6)GO TO 507
  IF(TEMP1.EQ.COM7)GO TO 508
  IF(TEMP1.EQ.COM8)XADJ=TEMP2
  IF(TEMP1.EQ.COM9)SGPRINT=.TRUE.
  IF(TEMP1.EQ.COM10)DPRINT=.TRUE.
  IF(TEMP1.EQ.COM11)SPPRINT=.TRUE.
  IF(TEMP1.EQ.COM12)EPRINT=.TRUE.
  IF(TEMP1.EQ.COM13)KPLOTD=.TRUE.
  IF(TEMP1.EQ.COM14)PLOTD=.TRUE.
  IF(TEMP1.EQ.COM15)PLOTN=.TRUE.
  IF(TEMP1.EQ.COM16)FRAME=.FALSE.
  IF(TEMP1.EQ.COM17)GO TO 511
  IF(TEMP1.EQ.COM18)PLOTSP=.TRUE.
  IF(TEMP1.EQ.COM19)KPLOTN=.TRUE.
  IF(TEMP1.EQ.COM20)RZERO=TEMP2
  IF(TEMP1.EQ.COM21)PRTABLE=.TRUE.
  IF(TEMP1.EQ.COM22)GO TO 510
  IF(TEMP1.EQ.COM23)PRSCAT=.TRUE.
  IF(TEMP1.EQ.COM24)PLOTP=.TRUE.
  IF(TEMP1.EQ.COM25)SIGMULT=TEMP2
  IF(TEMP1.EQ.COM26)GO TO 504
  GO TO 501
502 NO=TEMP2
  RHO=TEMP3
  IADJ=TEMP4
  MAT(1)=TEMP5
  MAT(2)=TEMP6
  CALL CENTER(MAT,2,MAT,20)
  DENS=RHO
  NELECT=0.0
  DO 5020 I=1,NO
  READ 102,(ZT(J,I),J=1,2),AT(I)
  ZT(2,I)=ZT(2,I)*1.0E22
5020 NELECT=NELECT+ZT(2,I)*ZT(1,I)
C   ZT(1,I)=ATOMIC NUMBER OF COMPONENT I
C   ZT(2,I)=ATOMIC DENSITY OF COMPONENT I, ATOMS PER CM**3 .
GO TO 501
503 Z=TEMP2
  IZ=IFIX(Z)
  A=TEMP3
```



```
BEAM(1)=TEMP5
BEAM(2)=TEMP6
CALL CENTER(BEAM,2,BEAM,20)
GO TO 501
504 NDTAPT=TEMP2
READ 105,(YDATA(I),XDATA(I),I=1,NDTAPT)
GO TO 501
506 E(1)=TEMP2
GO TO 501
507 CONST1=TEMP2
LNORM=1
ASSIGN 768 TO NNN1
GO TO 501
508 CONST2=TEMP2
ASSIGN 765 TO NNN2
GO TO 501
510 ASSIGN 768 TO NNN1
CONST1=TEMP2
LNORM=2
GO TO 501
511 READ(2,104)(XNAME(I),I=1,8)
CALL CENTER(XNAME,8,TITLE,43)
CALL CENTER(XNAME,8,XNAME,132)
GO TO 501
515 WRITE(3,103)(XNAME(I),I=1,13)
WRITE(3,111)
PRINT 112,(BEAM(I),I=1,2),IZ,A,E(1)
PRINT 113,CRIT1,FR,SIGMULT,RZERO
IF(XADJ.EQ.0.0)GO TO 516
WRITE (3,144) XADJ
GO TO 517
516 WRITE(3,143)
517 IF(LNORM.EQ.0)GO TO 518
IF(LNORM.EQ.1)WRITE(3,145)CONST1
IF(LNORM.EQ.2)WRITE(3,157)CONST1
GO TO 519
518 WRITE(3,146)
519 IF(CONST2.EQ.0.0)GO TO 520
WRITE(3,147)CONST2
520 WRITE(3,148)
PRINT 161,(MAT(I),I=1,2),RH0,IADJ
PRINT 162,NO
PRINT 163,(I,ZT(1,I),AT(I),ZT(2,I),I=1,NO)
```

C BEGIN CALCULATIONS

```
601 Z2=Z**2
DE=0.01*E(1)
CALL BEYE
FR2=FR/A
INT=0.0
SIGMA2=0.0
ATTEN(1)=1.0
SIGMA(1)=0.0
XBAR(1)=0.0
SBAR(1)=0.0
Y(1)=0.0
THETA2=0.0
```

```

TEMP9=DE*0.5*A
F(1)=DEX(E(1))
CROSS(1)=XSEC(E(1))
GG(1)=G(E(1))
DO 603 I=2,500
LET(I)=0.0
DELTA(E(I))=0.0
603 N(I)=0.0
N(1)=1.0
LET(1)=F(1)
IND(1)=JDEX1

```

C DELTA-FUNCTION APPROXIMATION CALCULATIONS

```

JREG=1
DO 615 I=2,500
IF(I.EQ.500)GO TO 900
E(I)=E(I-1)-DE
CROSS(I)=XSEC(E(I))
GG(I)=G(E(I))
F(I)=DEX(E(I))
SBAR(I)=SBAR(I-1)+TEMP9 *(1.0/F(I-1)+1.0/F(I))
INT=INT+TEMP9 *(CROSS(I-1)/F(I-1)+CROSS(I)/F(I))
ATTEN(I)=EXP(-INT)
SIGMA2=SIGMA2+TEMP9 *(GG(I-1)/(F(I-1))**3+GG(I)/(F(I))**3)
SIGMA(I)=SQRT(SIGMA2)*SIGMULI
N(I)=ATTEN(I)
LET(I)=N(I)*F(I)
IF(LET(I).LE.LET(I-1))GO TO 605
IKEEP=I
605 IND(I)=JDEX1
IF(CROSS(I)*SIGMA(I).GT.CRIT1)GO TO 620
TESTP2=ABS((F(I)-F(I-1))/DE)
IF(TESTP2*SIGMA(I).GT.A*CRIT1)GO TO 620
615 CONTINUE
620 I5=I

```

C NUMERICAL INTEGRATION SECTION

```

I6=I5+1
ASSIGN 641 TO NNN5
ASSIGN 630 TO NNN6
JREG=2
DO 643 J=I6,500
IF(J.EQ.500)GO TO 900
GO TO NNN6
630 IF(E(J-1).GT.10.0)GO TO 638
634 ASSIGN 639 TO NNN6
DE=0.2
GO TO 639
638 DE=FR2*SIGMA(J-1)*F(J-1)
IF((DE/E(J-1)).GT.0.05)DE=0.05*E(J-1)
639 E(J)=E(J-1)-DE
640 IF(E(J).LE.0.1)GO TO 646
CROSS(J)=XSEC(E(J))
GG(J)=G(E(J))
F(J)=DEX(E(J))
TEMP9=0.5*A*(E(J-1)-E(J))

```

```
SBAR(J)=SBAR(J-1)+TEMP9 *(1.0/F(J-1)+1.0/F(J))
GO TO NNN5
641 IF(SBAR(J)-SBAR(I5).LE.3.0*SIGMA(I5)) GO TO 642
    I7=J+1
    ASSIGN 642 TO NNN5
642 INT=INT+TEMP9 *(CROSS(J-1)/F(J-1)+CROSS(J)/F(J))
    ATTEN(J)=EXP(-INT)
    SIGMA2=SIGMA2+TEMP9 *(GG(J-1)/(F(J-1))**3+GG(J)/(F(J))**3)
643 SIGMA(J)=SQRT(SIGMA2)*SIGMULT
646 I8=J-1
    E(I8+1)=0.0
    DO 720 I=I7,I8
        IND(I)=JDEX2
        DO 713 J=I5,I8
713 U(J)=(SBAR(I)-SBAR(J))/SIGMA(J)
    U(I8+1)=U(I8)
    DO 715 J=I6,I8
        FACT=ATTEN(J)*M(U(J))
        FACT2=FACT*(U(J-1)-U(J+1))
        N(I)=N(I)+FACT2
715 LET(I)=LET(I)+FACT2*F(J)
    N(I)=N(I)/2.
    LET(I)=LET(I)/2.
716 IF(LET(I).GT.LET(I-1))IKEEP=I
720 CONTINUE
```

C CALCULATIONS BEYOND THE RANGE

```
DELTAS=0.1*SIGMA(I8)
I=I8
JREG=3
721 I=I+1
    IF(I.EQ.500)GO TO 900
    E(I)=0.0
    SBAR(I)=SBAR(I-1)+DELTAS
    ATTEN(I)=ATTEN(I-1)
    SIGMA(I)=SIGMA(I-1)
    IND(I)=JDEX3
    DO 722 J=I5,I8
722 U(J)=(SBAR(I)-SBAR(J))/SIGMA(J)
    U(I8+1)=U(I8)
    DO 725 J=I6,I8
        FACT=ATTEN(J)*M(U(J))
        FACT2=FACT*(U(J-1)-U(J+1))
        N(I)=N(I)+FACT2
725 LET(I)=LET(I)+FACT2*F(J)
    N(I)=N(I)/2.
    LET(I)=LET(I)/2.
    IF(LET(I).GT.LET(I-1))IKEEP=I
    TEMP11=LET(I)/LET(IKEEP)
    IF(TEMP11.GT.0.001) GO TO 721
    IMAX=I
```

C CALCULATE THE SPECTRUM AT THE BRAGG PEAK.....

```
DO 727 J=I5,I8
727 U(J)=(SBAR(IKEEP)-SBAR(J))/SIGMA(J)
    U(I8+1)=U(I8)
```

```
DO 728 J=I6,I8
FACT=ATTEN(J)*M(U(J))
DUDE(J)=(U(J-1)-U(J))/(E(J-1)-E(J))+(U(J)-U(J+1))/(E(J)-E(J+1))
728 SPECT2(J)=FACT*DUDE(J)
CALL SCATTER
```

C INTERNAL SHIFTING ROUTINE

```
JM=IMAX-I7
DO 730 K=0,JM
E(I6+K)=E(I7+K)
SBAR(I6+K)=SBAR(I7+K)
Y(I6+K)=Y(I7+K)
THETA(I6+K)=THETA(I7+K)
THETAS(I6+K)=THETAS(I7+K)
XBAR(I6+K)=XBAR(I7+K)
ATTEN(I6+K)=ATTEN(I7+K)
SIGMA(I6+K)=SIGMA(I7+K)
N(I6+K)=N(I7+K)
LET(I6+K)=LET(I7+K)
730 IND(I6+K)=IND(I7+K)
JM=I8-I7
DO 731 K=0,JM
731 SPECT2(I6+K)=SPECT2(I7+K)
KS1=I6
KS2=I6+I8-I7-1
IMAX=IMAX-I7+I6
IKEEP=IKEEP-I7+I6
```

C NUMBER DENSITY NORMALIZATION

```
GO TO NNN2
765 DO 766 J=1,IMAX
766 N(J)=N(J)*CONST2
767 GO TO NNN1
```

C LET NORMALIZATION

```
768 IF(LNORM.EQ.1)TEMP=CONST1/LET(IKEEP)
IF(LNORM.EQ.2)TEMP=CONST1/LET(1)
DO 769 I=1,IMAX
769 LET(I)=LET(I)*TEMP
```

C CALCULATION OF MEAN ENERGY AT BRAGG PEAK

```
770 IF(IKEEP.GT.15)GO TO 771
EMEAN=E(IKEEP)
GO TO 773
771 TEMP=0.0
DENOM=0.0
KS3=KS2-1
DO 772 J=KS1,KS3
XPP=0.5*SPECT2(J)*(E(J+1)+E(J-1))
TEMP=TEMP+XPP*E(J)
772 DENOM=DENOM+XPP
EMEAN=TEMP/DENOM
773 IF(XADJ.EQ.0.0)GO TO 775
```

C ROUTINE FOR ADJUSTING THE ABSCISSAS

```
TEMP5=XADJ-XBAR(IKEEP)
DO 774 I=1,IMAX
SBAR(I)=SBAR(I)+TEMP5
774 XBAR(I)=XBAR(I)+TEMP5
```

C BRAGG PEAK SPECTRUM NORMALIZATION

```
775 JM=KS1
K1=KS1+1
DO 776 J=K1,KS2
IF(SPECT2(J).GT.SPECT2(JM))JM=J
776 CONTINUE
DO 777 J=KS1,JM
COMP=SPECT2(J)/SPECT2(JM)
IF(COMP.GT.1.0E-4)GO TO 778
777 CONTINUE
778 KS1=J
TEM=SPECT2(JM)
DO 779 J=KS1,KS2
779 SPECT2(J)=SPECT2(J)/TEM
```

C ROUTINE TO CALCULATE BRAGG PEAK WIDTH AT HALF-MAXIMUM

```
780 TEMP=0.5*LET(IKEEP)
IT=IMAX-1
DO 781 J=1,IT
I=IMAX-J
781 IF(LET(I).GT.TEMP) GO TO 782
782 X1=(XBAR(I)-XBAR(I-1))*(LET(I-1)-TEMP)/(LET(I-1)-LET(I))
2+XBAR(I-1)
RANGE=X1
J1=J+5
DO 783 J=J1,IT
I=IMAX-J
783 IF(LET(I).LT.TEMP) GO TO 784
WIDTH=9.999E99
GO TO 786
784 X2=(XBAR(I)-XBAR(I-1))*(LET(I-1)-TEMP)/(LET(I-1)-LET(I))
2+XBAR(I-1)
WIDTH=X1-X2
```

C ROUTINE FOR CALCULATING TEN-PERCENT ORDINATE AND CORRESPONDING
C SCATTERING QUANTITIES.

```
786 TEMP=0.1*LET(IKEEP)
J1=IKEEP+1
DO 787 J=J1,IMAX
IF(LET(J).LT.TEMP)GO TO 788
787 CONTINUE
788 J10=J
FACTOR=(LET(J10-1)-TEMP)/(LET(J10-1)-LET(J10))
Y10=Y(J10-1)+(Y(J10)-Y(J10-1))*FACTOR
X1=SBAR(J10-1)+(SBAR(J10)-SBAR(J10-1))*FACTOR
X2=XBAR(J10-1)+(XBAR(J10)-XBAR(J10-1))*FACTOR
PD=100*(X1-X2)/X1
790 IF(EPRINT)CALL PRINTE(E,IMAX)
```

```

IF(SGPRINT)CALL PRINTG(IMAX,XBAR,ATTEN,SIGMA,E)
IF(DPRINT)CALL PRINTD(IMAX,XBAR,N,LET,IND)
IF(XADJ.NE.0.0)WRITE(3,149)TEMP5
IF(SPPRINT)CALL PRINTSP(KS1,KS2,E,SPECT2)

```

```

IF(PRSCAT)CALL PRSCATT
TEMP1=LET(IKEEP)/LET(1)
PRINT 107,TTDATE
WRITE(3,150){XNAME(I),I=1,13}
WRITE(3,151)TEMP1
WRITE(3,153)XBAR(IKEEP)
WRITE(3,154)EMEAN
WRITE(3,155)WIDTH
WRITE(3,156)RANGE
WRITE(3,158)PD
WRITE(3,159)Y10
WRITE(5) E(1),WIDTH,TEMP1,EMEAN,X1,XBAR(IKEEP),PD,Y10
IF(KPLOTD)CALL KWPLLOT(1)
IF(KPLOTN)CALL KWPLLOT(2)
IF(PRTABLE)CALL TABLE
IF(.NOT.PLOTD)GO TO 800
IF(FRAME)CALL CCNEXT
CALL GMPRINT(1)
800 IF(.NOT.PLOTN)GO TO 810
IF(FRAME)CALL CCNEXT
CALL GMPRINT(0)
810 IF(.NOT.PLOTSP)GO TO 1000
IF(FRAME)CALL CCNEXT
CALL GMPRINT(3)
GO TO 1000

```

C ERROR ABORT

```

900 PRINT 160,JREG,E(499)
IMAX=499
EPRINT=.TRUE.
SGPRINT=.TRUE.
DPRINT=.TRUE.
SPPRINT=.TRUE.
GO TO 790
1000 CONTINUE
CALL CCEND
RETURN

```

C FORMAT STATEMENTS

```

100 FORMAT(I10)
101 FORMAT(A10,3E10.4,2A10,2E10.0)
102 FORMAT(8E10.4)
103 FORMAT(15A10)
104 FORMAT(8A10)
105 FORMAT(2E10.0)
106 FORMAT(100X,A10)
107 FORMAT(1H1,///100X,A10)
110 FORMAT(///100X,A10///49X,33H-----PROGRAM BRAGG-----/)
111 FORMAT (/////////35X,61H-----INPUT DATA-----)

```

```

2----- -- - )
112 FORMAT(///22X,14HBEAM PARTICLES,12X,12HBEAM AT. NO. ,11X,12HBEAM A
    2T. WT. ,8X,19HBEAM INITIAL ENERGY
    3 //19X,2A10,14X,I2,17X,F7.2,17X,F8.2///)
113 FORMAT(27X,5HCRT1,21X,2HFR,          19X,7HSIGMULT,17X,5HRZERO//
    2 24X,E11.4,13X,E11.4,14X,F7.3,15X,E11.4///)
114 FORMAT (1H1)
119 FORMAT(22X,2(F9.3,11X,E11.4,18X))
141 FORMAT(A10,E12.5)
143 FORMAT(//22X,45HNO ADJUSTMENT OF THE ABSCISSAS HAS BEEN MADE )
144 FORMAT(//22X,50HALL ABSCISSAS ARE SHIFTED TO PUT THE BRAGG PEAK AT
    2,F7.3, 8HG/CM**2. )
145 FORMAT(//22X,37HTHE LET-DISTRIBUTION IS NORMALIZED TO ,E11.4,18H A
    2T THE BRAGG PEAK )
146 FORMAT(//22X,48HNO NORMALIZATION OF THE LET-DISTRIBUTION IS MADE )
147 FORMAT(//22X,48HTHE NUMBER-DENSITY DISTRIBUTION IS NORMALIZED TO ,
    2E11.4,24H AT THE INITIAL ORDINATE )
148 FORMAT(//22X,59HNO NORMALIZATION OF THE NUMBER-DENSITY DISTRIBUTIO
    2N IS MADE )
149 FORMAT(// 22X,35H ALL ABSCISSAS HAVE BEEN SHIFTED BY ,F8.4,
    2 8HG/CM**2. )
150 FORMAT (///55X,18HSUMMARY OF RESULTS//15A10///)
151 FORMAT(///30X,48H(BRAGG PEAK/INITIAL) DOSE RATIO.....
    2 , 2F9.4)
153 FORMAT(//30X,48HPENETRATION DEPTH AT BRAGG PEAK (G/CM**2)..... ,
    2F9.4)
154 FORMAT(//30X,48HAVERAGE ENERGY AT BRAGG PEAK (MEV/NUCLEON).....
    2F9.4)
155 FORMAT(//30X,48HBRAGG PEAK FULL WIDTH AT HALF-MAXIMUM.....
    2E10.3)
156 FORMAT(//30X,48HMEAN RANGE (G/CM**2).....,
    2F9.4)
157 FORMAT(//22X,37HTHE LET-DISTRIBUTION IS NORMALIZED TO E11.4,
    2 24H AT THE INITIAL ORDINATE )
158 FORMAT(//30X,48HPERCENTAGE DETOUR FACTOR..... ,
    2 F8.4)
159 FORMAT(//30X,48HMEAN LATERAL DISPLACEMENT OF BEAM (G/CM**2).....
    2 E10.3)
160 FORMAT(1H1//5X,82HPROBLEM ABORT.....VARIABLE STORAGE REQUIREMENTS
    2EXCEED ALLOWABLE LIMITS IN REGION I2//
    3 5X,28HFINAL CALCULATED ENERGY.....E11.4)
161 FORMAT(1H1//35X,41H----- -TARGET DATA----- ///
    2 30X,20HMATERIAL DESIGNATION,5X,16HSPECIFIC GRAVITY,8X,4HIADJ/
    3 30X,2A10,10X,F6.3,12X,F6.2)
162 FORMAT(//30X,44HNUMBER OF COMPONENTS IN TARGET MATERIAL.....I3///
    2 44X,6HATOMIC,5X,6HATOMIC,6X,12HATOM DENSITY /
    3 30X,9HCOMPONENT,5X,6HNUMBER,5X,6HWEIGHT,5X,15H(NO. PER CM**3)//)
163 FORMAT(33X,I2,10X,F3.0,6X,F7.3,7X,E11.4)
    END

```

FUNCTION XSEC(E)

C FUNCTION XSEC COMPUTES THE MACROSCOPIC CROSS SECTION FOR A
C MATERIAL COMPOSED OF ONE OR MORE ELEMENTS. A AND Z ARE THE AT.WT.
C AND AT. NO. OF THE BEAM, AND AT(I) AND ZT(1,I) ARE THE CORRESPON-
C DING QUANTITIES FOR THE MATERIAL. ZT(2,I) ARE THE SCALED ATOMIC
C DENSITIES FOR THE MATERIAL.

```
COMMON/GDATA2/RHO,RZERO
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO
XSEC=0.0
DO 100 I=1,NO
  IF(A.EQ.1.00)A3=0.0
  IF(A.NE.1.0)A3=A**0.333333
  BLAMBD=1.977E-11/(A*SQRT(1862.0*E+E**2))
  TEMP1=RZERO*1.0E-13*(A3 +AT(I)**0.333333+BLAMBD)
  TEMP2=A *AT(I)/(A +AT(I))
  TEMP3=1.437E-13*Z*ZT(1,I)
  TEMP4=TEMP3/(TEMP2*TEMP1*E)
  IF(TEMP4.GE.1.0)GO TO 50
  SIG=3.14159*(TEMP1**2)*(1.0-TEMP4)
  GO TO 51
50 SIG=0.0
51 XSEC=XSEC+SIG*ZT(2,I)
100 CONTINUE
XSEC=XSEC/RHO
RETURN
END
```


SUBROUTINE SCATTER

```

C
C SUBROUTINE SCATTER COMPUTES THE MEAN VALUES OF THE QUANTITIES
C (S-X) AND (Y) FOR ALL ENERGIES. IT THEN COMPUTES THE ARRAYS
C (X), N(X), AND LET(X)..... ALSO CALCULATED ARE THE ARRAYS OF
C THETA, THE MEAN ANGLE, AND THETAS, THE RATE OF CHANGE OF THE
C MEAN ANGLE.
C THE ROUTINE IS SUITABLE FOR SINGLE OR MULTIPLE COMPONENT TARGETS.
C Z=PARTICLE ATOMIC NUMBER
C A=PARTICLE ATOMIC WEIGHT
C ZM(I)=TARGET ATOMIC NUMBER, MATERIAL -I- .
C AM(I)=TARGET ATOMIC WEIGHT, MATERIAL -I- .
C
REAL INT1,INT2,INT3
COMMON/CHAIR/IADJ,Z,A,DENS,AM(10),ZT(2,10),NO
COMMON ATTEN(500),SBAR(500),E(500),SIGMA(500),IND(500),LET(500),
2 N(500),SPECT2(500),THETAS(500),THETA(500),XBAR(500),Y(500),
3 XDATA(300),YDATA(300),F(500)
COMMON/GMDATA1/IMAX,DIFF,I8,PD
COMMON/GDATA2/RHO,RZERO
REAL LET,N,NATOM(10)
DIMENSION TEMP1(10),TEMP2(10),ZM(10),TEMP3(10),GAMMA(10),THS(10)
DIMENSION SAVE(10), THETAS2(500)
EQUIVALENCE (THETAS2,THETAS)

INT1=0
INT2=0
INT3=0
THETA2=0.0
DIFF=0.0
Y(1)=0.0
THETA(1)=0.0
XBAR(1)=0.0
DO 10 J=1,NO
5 SAVE(J)=0.0
NATOM(J)=ZT(2,J)
ZM(J)=ZT(1,J)
GAMMA(J)=A/AM(J)
TEMP1(J)=(2.606E-25/RHO)*NATOM(J)*(Z*ZM(J)*(1.0+GAMMA(J))/A)**2
10 TEMP2(J)=(3.836E4)/(AM(J)*ZM(J))**0.333333
DO 300 I=1,I8
14 THETAS2(I)=0.0
DO 120 J=1,NO
TEMP5=842.2*A*SQRT(E(I)*(E(I)+1862.0))/((ZM(J)**0.333333)*
2(1.0+GAMMA(J)))
RATIO=AMIN1(TEMP5,TEMP2(J))
H=(E(I)*(E(I)+1862.0)/(E(I)+931.0))**2
TSCM2=(TEMP1(J)/H)*(ALOG((RATIO**2)+1.0)-1.0)
TSCM=SQRT(TSCM2)
THS(J)=ATAN2(SIN(TSCM),COS(TSCM)+GAMMA(J))
11 IF(THS(J).GE.SAVE(J))GO TO 12
THS(J)=THS(J)+3.14159265
GO TO 11
12 SAVE(J)=THS(J)
120 THETAS2(I)=THETAS2(I)+THS(J)**2
IF(I.EQ.1)GO TO 300
28 DELTAE=E(I-1)-E(I)
TEMP=DELTAE*0.5*A
32 THETA2=THETA2+TEMP*(THETAS2(I-1)/F(I-1)+THETAS2(I)/F(I))

```

```
THETA(I)=SQRT(THETA2)
IF(THETA(I).LT.0.785398)GO TO 31
IN=I
GO TO 302
31 DIFF=DIFF+TEMP*((1.0-COS(THETA(I-1)))/F(I-1)
2 +(1.0-COS(THETA(I)))/F(I))
XBAR(I)=SBAR(I)-DIFF
T1=(THETAS2(I-1)/COS(THETA(I-1))**2)/F(I-1)
T2=(THETAS2(I)/COS(THETA(I))**2)/F(I)
INT1=INT1+TEMP*(T1+T2)
INT2=INT2+TEMP*(XBAR(I-1)*T1+XBAR(I)*T2)
INT3=INT3+TEMP*((XBAR(I-1)**2)*T1+(XBAR(I)**2)*T2)
YSQ=(XBAR(I)**2)*INT1-2*XBAR(I)*INT2+INT3
Y(I)=SQRT(YSQ)
300 CONTINUE
C
C CALCULATIONS BEYOND THE RANGE
C
IN=I8+1
302 DO 400 I=IN,IMAX
DS2=(SBAR(I)-SBAR(I-1))*0.70711
Y(I)=Y(I-1)+DS2
XBAR(I)=XBAR(I-1)+DS2
THETA(I)=0177700000000000 00
400 THETAS(I)=0177700000000000 0000
IN1=IN-1
DO 405 I=1,IN1
405 THETAS(I)=SQRT(THETAS2(I))
RETURN
END
```

```

SUBROUTINE BEYE
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
COMMON/GEN/LI,LAZ,NN,II,IEV,ANL
COMMON/TABLE/ZEX,EV,R
COMMON/ABLOK/AMN(3,3),ALPHA(4,4)/BBLOK/CE(10),CN(10),CN1(10),
1DEN(10)/CBLOK/B(5)
DIMENSION EV(200),ZEX(200)
DIMENSION DR(22),TABLE(22,10),          BETA(3),EL(3),D(6,5)
1,IL(5),EQ(22)
REAL IADJ,LI,LAZ,LE,LL,LAMB2,LAMBDA
DATA EQ/.01,.015,.02,.03,.04,.05,.07,.1,.15,.2,.3,.4,.5,.7,1.0,1.5
1,2.0,3.,4.,5.,7.,10./,TABLE/183.,230.,265.,320.,360.,390.,430.,440
2.,410.,380.,330.,290.,265.,230.,172.,131.,109.,83.,69.,58.,45.,34.
3279.,118.,141.,164.,205.,235.,260.,285.,315.,325.,320.,290.,270.,
4250.,220.,170.,131.,109.,83.,69.,58.,45.,34.279,95.,114.,132.,164.
5,187.,208.,230.,254.,264.,263.,243.,230.,216.,193.,156.,124.,105.,
681.6,68.,58.,45.,34.279,71.,86.,99.,122.,140.,155.,175.,193.,203.,
7206.,196.,189.,181.,166.,142.,117.,101.,80.,67.,57.,45.,34.279,
848.,58.,66.,80.,93.,103.,120.,132.,142.,149.,150.,149.,147.,140.,
9129.,111.,98.,79.,67.,57.,45.,34.279,39.,47.,54.,65.,75.,83.,97.,1
*11.,123.,130.,133.,133.,131.,128.,120.,107.,94.,78.,66.,57.,45.,
134.279,34.,40.,47.,56.,64.,71.,82.,94.,108.,112.,121.,122.,122.,
2120.,111.,100.,90.,75.,64.,56.,44.,34.279,28.,33.,38.,47.,54.,60.,
369.,80.,92.,100.,109.,110.,111.,110.,107.,95.,86.,73.,62.,55.,43.,
434.279,23.,27.,32.,39.,46.,51.,59.,69.,80.,87.,96.,100.,101.,101.,
598.,90.,81.,70.,60.,54.,42.,34.279,19.,23.,27.,32.,38.,43.,50.,60.
6,70.,77.,87.,91.,93.,94.,90.,84.,76.,67.,58.,52.,41.,34.279/
DATA AMN/
6 -.312.,.18664E-1,-.24598.,.11548,-.99661E-2/,ALPHA/
7 -.80155E1,.36916,-.14307E-1,.34718E-2,.18371E1,-.1452E-1,
8 -.30142E-1,.23603E-2,.45233E-1,-.95873E-3,.71303E-2,-.68538E-3,
9 -.59898E-2,-.52315E-3,-.33802E-3,.39405E-4/,D/30*0./
100 IF(IADJ.EQ.0.) GO TO 999
    IF (NO.GT.1) GO TO 20
    NO=1
    DEN(1)=1.
    DENS=1.
C ZT(1,I) ARE THE AT. NOS. OF THE TARGETS.
C ZT(2,I) ARE THE RELATIVE ATOMIC ABUNDANCES OF THE TARGETS
    GO TO 54
20 SAT=0.0
    DO 51 I=1,NO
51 SAT=SAT+ZT(2,I)*AT(I)
    DO 52 I=1,NO
52 DEN(I)=ZT(2,I)*DENS*AT(I)/SAT
    SUM=0.
    DO 53 I=1,NO
53 SUM=SUM +ZT(1,I)*DEN(I)/AT(I)
    ZAF=SUM /DENS
    GO TO 55
54 ZAF=ZT(1,1)/AT(1)
55 LI=ALOG(IADJ)
    LAZ=ALOG(1./ZAF)
    IF(Z.GT.10.) GO TO 500
C Z LESS THAN 11
C LOW ENERGY DEDX
    NN=0
    R2=DIDX(2.)/112.3138
    R10=DIDX(10.)/34.279

```

```

Q=ALOG(R10/R2)/ALOG(5.)
P=R2/(2.**Q)
Z23=Z**(2./3.)
IF(NO.EQ.1)GO TO 403
SUM=0.
DO 402 I=1,NO
SUM=SUM+DEN(I)*ZT(1,I)/(DENS*AT(I)*(Z23+ZT(1,I)**(2./3.))**1.5)
402 CONTINUE
F=2.08*(Z23+5.54)**1.5*SUM
GO TO 404
403 F=2.08*ZAF*((Z23+5.54)/(Z23+ZT(1,1)**(2./3.))**1.5)
404 EP=(F/P)**(1./Q)
EP=AMINI(EP,10.)
DO 406 I=1,21
EV(I)=EQ(I)
E=EV(I)
IF(EP.LE.E) GO TO 405
DR(I)=F
GO TO 406
405 DR(I)=P*E**Q
406 CONTINUE
JK=Z
Z2=Z**2
DO 407 I=1,21
ZEX(I)=DR(I)*TABLE(I,JK)*Z2
407 CONTINUE
C SET UP TABLE
EV(22)=10.
EV(23)=10.4
I=23
DO 408 J=12,50,2
I=I+1
408 EV(I)=J
DO 409 J=55,200,5
I=I+1
409 EV(I)=J
DO 410 J=210,1000,10
I=I+1
410 EV(I)=J
IEV=I
C HIGH ENERGY DEDX
DO 411 I=22,IEV
ZEX(I)=Z2*DIDX(EV(I))
411 CONTINUE
GO TO 201
C Z GREATER THAN 10
C DEFINE ENERGY REGION BOUNDARIES AND SET UP TABLE
500 BETA(1)=(Z**(1./3.)/137. )**2
BETA(2)=2./465.5
BETA(3)=(3.*Z/137. )**2
DO 503 I=1,3
IF(BETA(I).GT..01) GO TO 501
EL(I)=465.5*BETA(I)
GO TO 503
501 IF(BETA(I).GT..9999) GO TO 502
GAMMA=1./SQRT(1.-BETA(I))
EL(I)=931.*(GAMMA-1.)
GO TO 503

```

```
502 EL(I)=1.E10
503 CONTINUE
    EV(1)=.01
    EV(2)=.015
    DO 540 I=2,9
540 EV(I+1)=.01*FLOAT(I)
    EV(11)=.1
    EV(12)=.15
    EV(13)=.2
    EV(14)=.3
    EV(15)=.4
    EV(16)=.437
    EV(17)=.489
    EV(18)=.5
    EV(19)=.6
    EV(20)=.613
    EV(21)=.7
    EV(22)=.8
    EV(23)=.816
    EV(24)=1.
    EV(25)=1.12
    EV(26)=1.5
    JL=26
    DO 541 I=2,10
    JL=JL+1
541 EV(JL)=I
    EV(36)=10.4
    I=36
    DO 504 J=12,50,2
    I=I+1
504 EV(I)=J
    DO 505 J=55,200,5
    I=I+1
505 EV(I)=J
    DO 506 J=210,1000,10
    I=I+1
506 EV(I)=J
    IEV=I
    DO 507 I=1,IEV
    JK=I
    IF(EV(I).GE.EL(1)) GO TO 507
507 CONTINUE
508 GO TO 900
509 IEL1=JK
    DO 510 I=JK,IEV
    JL=I
    IF(EV(I).GE.EL(2)) GO TO 512
510 CONTINUE
511 GO TO 901
512 IEL2=JL
    IF(EL(3).GE.EV(IEV)) GO TO 516
    DO 513 I=JL,IEV
    JK=I
    IF(EV(I).GE.EL(3)) GO TO 515
513 CONTINUE
514 GO TO 902
515 IEL3=JK-1
    GO TO 517
```

```

516 IEL3=IEV
517 CONTINUE
C LOW ENERGY REGION
Z23=Z**(2./3.)
Z876=7.39E4*Z**1.207
AOZ=A/Z
DO 518 I=1,NO
ZS23=Z23+ZT(1,I)**(2./3.)
ZTOAT=ZT(1,I)/AT(I)
AS=A+AT(I)
CE(I)=Z876*ZTOAT/ZS23**1.5
CN(I)=4.14281E6*(A/AS)**1.5*SQRT(Z*ZTOAT)/ZS23**.75
CN1(I)=45.1671*(AOZ/(ZTOAT*AS))**.27719/ZS23**.138595
518 CONTINUE
NN=1
ZEX(1)=DEDXL(EV(1))
DO 520 I=2,IEL1
ZEX(I)=DEDXL(EV(I))
520 CONTINUE
C MEDIUM-LOW ENERGY REGION
SPL=DEDXL(EV(IEL1))
SQREL=SQRT(EV(IEL1))
SQRREL=EV(IEL1)**.22281
CL=ALOG(SPL)
SUM=0.
DO 521 I=1,NO
EXPN=EXP(CN1(I)*EV(IEL1)**.27719)
SUM=SUM+(.5*(CE(I)+CN(I)/EXPN)/SQREL-.27719*CN(I)*CN1(I)/SQRREL/EX
1PN)*DEN(I)
521 CONTINUE
DSPL=SUM/DENS
DCL=DSPL/SPL
Z2=Z**2
RAT=RATIO(EV(IEL2))
RATSQ=RAT**2
DEX=DIDX(EV(IEL2))
SPH=Z2*RATSQ*DEX
CH=ALOG(SPH)
BEL=SQRT(EV(IEL2)/465.5)
IF (BEL.LE.Z23/137.) GO TO 522
DRAT=ANL/EV(IEL2)*(1.-45.7*IEL*ALOG(Z)/(2.*Z-Z23))
GO TO 523
522 DRAT=ANL/EV(IEL2)
523 CONTINUE
IF (EV(IEL2).LT.7.) GO TO 535
SUM1=0.
DO 526 M=1,4
SUM1=SUM1+ALPHA(M,3)*LI**(M-1)
526 CONTINUE
SUM=0.
DO 527 M=1,4
SUM=SUM+ALPHA(M,4)*LI**(M-1)
527 CONTINUE
DPDE=2./EV(IEL2)*(SUM1+3.*ALOG(EV(IEL2))*SUM)
GO TO 537
535 SUM=0.
DO 536 M=1,3
SUM=SUM+AMN(M,3)*LI**(M-1)

```

```

536 CONTINUE
    DPDE=2./EV(IEL2)*SUM
537 CONTINUE
    XLAM=LAMBDA(EV(IEL2))
    DXLAM=DEX*XLAM
    DCH=DRAT /RAT +1./EV(IEL2)-1./DXLAM-DXLAM/EV(IEL2)*DPDE
    ALE1=ALOG(EV(IEL1))
    IF(ALE1.EQ.0.) ALE1=.001
    DO 528 I=1,4
    D(1,I)=ALE1**(I-1)
528 CONTINUE
    ALE2=ALOG(EV(IEL2))
    IF(ALE2.EQ.0.) ALE2=.001
    DO 529 I=1,4
    D(2,I)=ALE2**(I-1)
529 CONTINUE
    DO 530 I=1,4
    D(3,I)=FLOAT(I-1)*ALE1**(I-2)
530 CONTINUE
    DO 531 I=1,4
    D(4,I)=FLOAT(I-1)*ALE2**(I-2)
531 CONTINUE
    D(1,5)=CL
    D(2,5)=CH
    D(3,5)=DCL*EV(IEL1)
    D(4,5)=DCH*EV(IEL2)
    CALL GLSQ(D,B,IL,4,4,SSSQ,0.,0.)
    K=IEL1+1
    NN=2
    DO 532 I=K,IEL2
    ZEX(I)=1./SPIML (EV(I))
532 CONTINUE
C MEDIUM-HIGH ENERGY REGION
    K=IEL2+1
    NN=3
    DO 546 I=K,IEL3
    II=I
    ZEX(I)=Z2*RATIO(EV(I))*2*DIDX(EV(I))
546 CONTINUE
    IF (IEL3.EQ.IEV) GO TO 201
    K=IEL3+1
C HIGH ENERGY REGION
    DO 534 I=K,IEV
    ZEX(I)=Z2 *DIDX(EV(I))
534 CONTINUE
C OUTPUT AND GO TO THE NEXT PROBLEM
    RETURN
C DIAGNOSTICS AND SKIP TO THE NEXT PROBLEM
900 WRITE(3,351)
351 FORMAT(////,31H STATEMENT 508 WAS ENCOUNTERED. )
    RETURN
901 WRITE(3,352)
352 FORMAT(////,31H STATEMENT 511 WAS ENCOUNTERED. )
    RETURN
902 WRITE(3,353)
353 FORMAT(////,31H STATEMENT 514 WAS ENCOUNTERED. )
    RETURN
999 PRINT 1112

```

```
1112 FORMAT(5X,27HPROBLEM ABORT.....IADJ=0.0 )
201 RETURN
END
```



```
FUNCTION DIDX(E)
REAL IADJ,LI,LE,LAMBDA
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
COMMON/GEN/LI,LAZ,NN,II,IEV,ANL
COMMON/ABLOK/AMN(3,3),ALPHA(4,4)
LE=ALOG(E)
IF(LE.EQ.0.) LE=.001
IF(E.LT.7.) GO TO 221
IF((E.EQ.7.).AND.(II.EQ.32)) GO TO 221
SUM=0.
DO 220 N=2,4
DO 220 M=1,4
SUM=SUM+FLOAT(N-1)*ALPHA(M,N)*(LI**(M-1))*(LE**(N-2))
220 CONTINUE
DIDX=E/(SUM*LAMBDA(E))
RETURN
221 SUM=0.
DO 223 N=2,3
DO 223 M=1,3
SUM=SUM+FLOAT(N-1)*AMN(M,N)*(LI**(M-1))*(LE**(N-2))
223 CONTINUE
DIDX=E/(SUM*LAMBDA(E))
IF (E.LT.1.) GO TO 224
RETURN
224 WRITE(3,1) E
1 FORMAT(37H ENERGY IN DEDX IS OUT OF RANGE      E=E15.8)
RETURN
END
```

```
FUNCTION DEDX(X)
COMMON/TABLE/YDATA(200),XDATA(200),R
COMMON/GEN/DUM(4),IMAX
M=IMAX
L1=1
L2=M
K=1
IF(X-XDATA(1))1,15,3
3 K=M
IF(XDATA(M)-X)1,15,9
9 K=M/2
IF(X-XDATA(K))20,15,29
20 L2=K
GO TO 23
29 L1=K
23 IF(L2-L1-1)1,14,25
25 M=L1+L2
GO TO 9
14 DEDX= YDATA(L1)+ (X-XDATA(L1))* (YDATA(L2)-YDATA(L1))/
2 (XDATA(L2)-XDATA(L1))
RETURN
15 DEDX=YDATA(K)
RETURN
1 DEDX=0.0
WRITE(3,7777)L1,L2,K,M
7777 FORMAT(2X,36HERROR IN FUNCTION DEDX...JOB ABORTED /(10X,18))
CALL EXIT
END
```

```

SUBROUTINE GLSQ(A,X,IL,N,M,ALPHA,E1,E2)
DIMENSION A(6,5), X(5), IL(5)
MM=M+1
LL=1
DO 60J=1,MM
60  IL(J)=0
    I=1
    DO 3K=1,MM
        II=I+1
        DO 4J=II,N
            IF (ABS(A(J,K))-E1) 4,4,6
6         T1=SQRT ((A(J,K))**2+(A(I,K))**2)
            S=A(J,K)/T1
            C=A(I,K)/T1
            DO 5L=K,MM
                T2=C*A(I,L)+S*A(J,L)
                A(J,L)=-S*A(I,L)+C*A(J,L)
5         A(I,L)=T2
            LL=LL+1
4         CONTINUE
            IF (ABS (A(I,K))-E2) 3,3,8
8         IL(K)=I
            I=I+1
3         CONTINUE
            X(MM)=-1.0
            II=M
            DO 35I=1,M
35        X(I)=0.
            DO 30J=1,M
                IF (IL(II)) 30,30,31
31        S=0.
                LL=II+1
                I=IL(II)
                DO 32K=LL,MM
32        S=S+A(I,K)*X(K)
                X(II)=-S/A(I,II)
30        II=II-1
                IF (IL(MM)) 50,51,50
51        ALPHA=0.
                GO TO 52
50        I=IL(MM)
                ALPHA=A(I,MM)
52        RETURN
    END
```

```
FUNCTION RATIO(E)
COMMON/GEN/LI,LAZ,NN,II,IEV,ANL
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
DIMENSION AN(5)
DATA AN/.413253,1.63475,10.4782,2.21626,.847578/
Z23=Z**(2./3.)
IF (E.LE.4.65) GO TO 200
BETA=SQRT(1.-1./(E/931.+1.)**2)
GO TO 201
200 BETA=SQRT(E/465.5)
201 IF (BETA.LE.Z23/137.) GO TO 202
IF (BETA.GE.2.*Z/137.) GO TO 204
G=(137.*BETA+4.*Z-3.*Z23)/(6.*Z-3.*Z23)
GO TO 203
202 G=2./3.
GO TO 203
204 G=1.
203 X=137.*BETA/Z**G
A1=AN(1)*X**(AN(2)**2)
A2=AN(3)*X**AN(4)
A3=AN(5)+1.
RATIO=1.-EXP(-A1)/A3-AN(5)/A3/(A2+1.)
IF(NN.EQ.1)ANL=A1*AN(2)**2*EXP(-A1)/A3+A2*AN(4)*AN(5)/A3/(A2+1.)**
12
IF((E.LT.1.5).OR.(BETA.GT.3.5*Z/137.))GO TO 205
RETURN
205 WRITE(3,1) E
1 FORMAT(37H ENERGY IN RATIO IS OUT OF RANGE E=E15.8)
RETURN
END
```

```
FUNCTION SPIML(E)
COMMON/GEN/LI,LAZ,NN,II,IEV,ANL
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
COMMON/CBLOK/B(5)
BETA1=Z**(1./3.)/137.**2
BETA2=2.5/465.5
IF (E.EQ.1.) GO TO 251
XLE=ALOG(E)
SUM=0.
DO 250 I=1,4
SUM=SUM+B(I)*XLE**(I-1)
250 CONTINUE
SPIML=1./EXP(SUM)
IF (E.LT.4.65)GO TO 253
BEL=1.-1./(E/931.+1.)**2
IF ((BEL.GT.BETA2).OR.(BEL.LT.BETA1)) GO TO 252
RETURN
253 BEL=E/465.5
IF ((BEL.GT.BETA2).OR.(BEL.LT.BETA1)) GO TO 252
RETURN
251 SPIML=1./EXP(B(1))
IF ((.002148.GT.BETA2).OR.(.002148.LT.BETA1)) GO TO 252
RETURN
252 WRITE(3,1) E
1 FORMAT(37H ENERGY IN SPIML IS OUT OF RANGE E=E15.8)
RETURN
END
```

```
FUNCTION DEDXL(E)
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
COMMON/GEN/LI,LAZ,NN,II,IEV,ANL
COMMON/BBLOK/CE(10),CN(10),CN1(10),DEN(10)
SUM=0.
SQRE=SQRT(E)
SQRRE=E**0.27719
DO 230 I=1,NO
SUM=SUM+(CE(I)+CN(I)/EXP(CN1(I)*SQRRE))*SQRE*DEN(I)
230 CONTINUE
DEDXL=SUM/DENS
BETA=Z/137.**2
IF (E.LT.4.65) GO TO 231
BEL=1.-1./(E/931.+1.)**2
IF (BEL.GT.BETA) GO TO 232
RETURN
231 BEL=E/465.5
IF (BEL.GT.BETA) GO TO 232
RETURN
232 WRITE(3,1) E
1 FORMAT(38H ENERGY IN DEDXL IS OUT OF RANGE E=E15.8)
RETURN
END
```

```
REAL FUNCTION LAMBDA(E)
REAL IADJ,LAZ,LI,LE,LL
COMMON/GEN/LI,LAZ,NN,II,IEV,ANL
COMMON/CHAIR/IADJ,Z,A,DENS,AT(10),ZT(2,10),NO,DUMMM(2)
COMMON/ABLOK/AMN(3,3),ALPHA(4,4)
LE=ALOG(E)
IF(LE.EQ.0.) LE=.001
IF(E.LT.7.) GO TO 221
IF((E.EQ.7.).AND.(II.EQ.32)) GO TO 221
SUM=0.
DO 210 N=1,4
DO 210 M=1,4
SUM=SUM+ALPHA(M,N)*(LI**(M-1))*(LE**(N-1))
210 CONTINUE
LL=LAZ+SUM
LAMBDA=EXP(LL)
RETURN
221 SUM=0.
DO 222 N=1,3
DO 222 M=1,3
SUM=SUM+AMN(M,N)*LI**(M-1)*(LE**(N-1))
222 CONTINUE
LL=LAZ+SUM
LAMBDA=EXP(LL)*.001
IF (E.LT.1.)GO TO 211
RETURN
211 WRITE(3,1) E
1 FORMAT(39H ENERGY IN LAMBDA IS OUT OF RANGE E=E15.8)
RETURN
END
```

SUBROUTINE KWPLOT(KK)

C SUBROUTINE KWPLOT SETS UP THE DESIRED ARRAY FOR QUICKPLOTING

```
DIMENSION TITLE(15),SET2(500)
COMMON ATEN(500),SBAR(500),E(500),SIGMA(500),IND(500),LET(500),
2 N(500),SPECT2(500),THETAS(500),THETA(500),XBAR(500),Y(500),
3 XDATA(300),YDATA(300),F(500)
EQUIVALENCE (SET2,Y)
COMMON/GMDATA1/IMAX,DIFF,I8,PD
COMMON/DATA/NDTAPT,IPLOTP
COMMON /GMDATA2/TITLE,IFRAME,INNP,KS1,KS2
REAL N,LET

IF(KK.EQ.1)GO TO 20
IF(KK.EQ.2)GO TO 30
20 DO 21 I=1,NDTAPT
21 SET2(I)=XINTERP(XDATA(I),XBAR,LET,IMAX)
GO TO 50
30 DO 31 I=1,NDTAPT
31 SET2(I)=XINTERP(XDATA(I),XBAR,N,IMAX)
50 CALL YGRAPH(NDTAPT,XDATA,YDATA,SET2)
RETURN
END
```



```
FUNCTION XINTERP(X,XDATA,YDATA,IMAX )
C
C   FUNCTION XINTERP INTERPOLATES WITHIN A SET OF DATA POINTS
C   XDATA(I), YDATA(I), I=1,IMAX. THE QUANTITY X IS THE GIVEN
C   VALUE OF THE INDEPENDENT VARIABLE, AND XINTERP IS THE INTERPOLATED
C   VALUE OF THE DEPENDENT VARIABLE.
C
  DIMENSION XDATA(1),YDATA(1)
  M=IMAX
  L1=1
  L2=M
  K=1
  IF(X-XDATA(1))1,15,3
3  K=M
  IF(XDATA(M)-X)8,15,9
  9  K=M/2
  IF(X-XDATA(K))20,15,29
20 L2=K
  GO TO 23
29 L1=K
23 IF(L2-L1-1)1,14,25
25 M=L1+L2
  GO TO 9
14 XINTERP= YDATA(L1)+ (X-XDATA(L1))* (YDATA(L2)-YDATA(L1))/
  2 (XDATA(L2)-XDATA(L1))
  RETURN
15 XINTERP=YDATA(K)
  RETURN
  1 XINTERP=YDATA(1)
  RETURN
  8 XINTERP=YDATA(IMAX)
  RETURN
  END
```

```

SUBROUTINE YGRAPH(M,X,Y,YFIT)
DIMENSION X(1) ,Y(1),YFIT(1)
DATA IFFF,IBBB,I000,IPPP/1HF,1H ,1HO,1HP/
YMIN=Y(1)
YMAX=Y(1)
DO 3 I=1,M
IF(YMIN .GT. Y(I)) YMIN=Y(I)
IF(YMAX .LT. Y(I)) YMAX=Y(I)
IF (YMIN .GT. YFIT(I)) YMIN=YFIT(I)
IF (YMAX .LT. YFIT(I)) YMAX=YFIT(I)
3 CONTINUE
WRITE (3,1005) YMIN,YMAX
1005 FORMAT (1H1,15X,E13.5,87X,E13.5/19X,101HIIIIIIIIIIIIIIIIIIIIIIIIIIIIII
1IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII
1IIIIIIIIII )
DO 1100 I=1,M
IO=1.0+100.0*(Y(I)-YMIN)/(YMAX-YMIN)
IO=MAX0(MINO(IO,100),1)
IP=1.0+100.0*(YFIT(I)-YMIN)/(YMAX-YMIN)
IP=MAX0(MINO(IP,100),1)
IF (IO .NE. IP) GO TO 1030
1008 IF (IO .NE. 1) GO TO 1020
WRITE(3,1010)X(I),IFFF
1010 FORMAT (1X,E13.5,6H --,100A1)
GO TO 1100
1020 K=IO-1
WRITE (3,1010) X(I), (IBBB,J=1,K),IFFF
GO TO 1100
1030 IPP=IPPP
IOO=I000
IF (IP .GT. IO) GO TO 1040
IPP=I000
IOO=IPPP
IDUMMY=IO
IO=IP
IP=IDUMMY
1040 IF (IO .GT. 1) GO TO 1060
K=IP-IO-1
IF (K .GT. 0) GO TO 1050
WRITE (3,1010) X(I), IOO,IPP
GO TO 1100
1050 CONTINUE
WRITE (3,1010) X(I), IOO,(IBBB,J=1,K),IPP
GO TO 1100
1060 K1=IO-1
K2=IP-IO-1
IF (K2 .GT. 0) GO TO 1070
WRITE(3,1010)X(I),(IBBB,J=1,K1),IOO,IPP
GO TO 1100
1070 CONTINUE
WRITE (3,1010) X(I), (IBBB,J=1,K1),IOO,(IBBB,J=1,K2),IPP
1100 CONTINUE
WRITE (3,1110) YMIN,YMAX
1110 FORMAT (19X,101HIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII
1IIIII!IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII /16X,E13.5,87
2X,E13.5)
WRITE (3,1120)
1120 FORMAT (33HOP REPRESENTS THE PREDICTED POINT/28HOO REPRESENTS THE
1DATA POINT/73HOF REPRESENTS BOTH THE DATA AND THE PREDICTED POINTS

```

2 IF THEY LIE TOGETHER)
RETURN
END

SUBROUTINE PRINTE(E,IMAX)
DIMENSION E(1)

C PRINTOUT SUBROUTINE FOR ENERGIES

116 FORMAT (1H1//16X,92H-----
2EV/NUCLEON)-----
117 FORMAT (25X,4(9X,F9.3))

ENERGIES (M

//)

10099 I=1
10100 IF(I-1+200-IMAX)10101,10113,10113
10101 WRITE(3,116)
DO10102J=1,50
K=I+J
10102 WRITE(3,117)(E(K-1),E(K+49),E(K+99),E(K+149))
I=I+200
GO TO 10100
10113 WRITE(3,116)
LP=(IMAX-I+1)/50
LC=(IMAX-I+1)-50*LP
LD=LC+1
IF(LC)10104,10103,10104
10103 L=LP
LC=50
GO TO(1001,10033,10043,10044),L
10104 L=LP+1
GO TO (1001,1002,1003,1004),L
1001 DO 10011 J=1,LC
K=I+J
10011 WRITE(3,117)(E(K-1))
GO TO 10046
1002 DO 10021 J=1,LC
K=I+J
10021 WRITE(3,117)(E(K-1),E(K+49))
LD=LC+1
10023 DO 10022 J=LD,50
K=I+J
10022 WRITE(3,117)(E(K-1))
GO TO 10046
1003 DO10031 J=1,LC
K=I+J
10031 WRITE(3,117)(E(K-1),E(K+49),E(K+99))
10033 DO 10032 J=LD,50
K=J+I
10032 WRITE(3,117)(E(K-1),E(K+49))
GO TO 10046
1004 DO10041 J=1,LC
K=I+J
10041 WRITE(3,117)(E(K-1),E(K+49),E(K+99),E(K+149))
10043 DO 10042 J=LD,50
K=I+J
10042 WRITE(3,117)(E(K-1),E(K+49),E(K+99))
GO TO 10046
10044 DO 10045 J=LD,50
K=I+J
10045 WRITE (3,117)(E(K-1),E(K+49),E(K+99),E(K+149))
10046 RETURN
END

```
SUBROUTINE PRINTG(IMAX,XBAR,ATTEN,SIGMA,E)
DIMENSION XBAR(1),ATTEN(1),SIGMA(1),E(1)
```

C PRINT SUBROUTINE FOR DISTANCES,ATTENUATION FACTORS,SIGMAS,ENERGIES

```
130 FORMAT(1H1//27X,11HPENETRATION,13X,8HSURVIVAL,7X, 20HMEAN SQUAR
2E STRAGGLE,11X,6HENERGY/24X,18HDISTANCE (G/CM**2),9X,8HFRACTION
3 8X,19HPARAMETER (G/CM**2),8X,13H(MEV/NUCLEON) ///)
131 FORMAT(27X,E11.4,11X,E11.4,10X,E11.4,13X,F9.3)
```

```
      I=1
210 IF(I.GE.IMAX)GO TO 214
211 IF((2+49).GT.IMAX)GO TO 214
212 WRITE(3,130)
      DO 213 J=1,50
      K=I+J
213 WRITE(3,131)(XBAR(K-1),ATTEN(K-1),SIGMA(K-1),E(K-1))
      I=50 +I
      GO TO 210
214 WRITE(3,130)
      DO 215 J=I,IMAX
215 WRITE(3,131)(XBAR(J),ATTEN(J),SIGMA(J),E(J))
216 RETURN
      END
```

```
SUBROUTINE PRINTD(IMAX,XBAR,N,LET,IND)
REAL N,LET
DIMENSION XBAR(1),LET(1),N(1),IND(1)
```

C PRINT SUBROUTINE FOR DISTANCES,FLUXES,LET-S

```
120 FORMAT(1H1//27X,11HPENETRATION,12X,13HPARTICLE FLUX,10X,
214HENERGY RELEASE,12X,11HCALCULATION/24X,17HDISTANCE(G/CM**2),6X,
318H(NUMBER/SEC-CM**2),8X,134(MEV-CM**2/G),16X,4HMODE///)
121 FORMAT(27X,E11.4,12X,E11.4,12X,E11.4,18X,A6)
```

```
I=1
200 IF(I.GE.IMAX)GO TO 204
201 IF((I+49).GT.IMAX)GO TO 204
202 WRITE(3,120)
DO 203 J=1,50
K=I+J
203 WRITE(3,121)(XBAR(K-1 ),N(K-1 ),LET(K-1 ),IND(K-1))
I=I+50
GO TO 200
204 WRITE(3,120)
DO 205 J=I,IMAX
205 WRITE(3,121)(XBAR(J),N(J),LET(J),IND(J))
230 RETURN
END
```

```

SUBROUTINE PRINTSP(KS1,KS2,E,SPECT2)
DIMENSION E(1),SPECT2(1)

```

C SPECTRAL PRINTOUT SUBROUTINE

```

136 FORMAT(1H1//20X,78H----- -- ENERGY SPECTRUM AT BRAG
2G PEAK----- ///21X,2(15HPARTICLE ENERGY,7X,
38HRELATIVE,13X)/22X,2(13H(MEV/NUCLEON),5X,14HNUMBER DENSITY,11X)
4//)
137 FORMAT(22X,2(F9.3,10X,E11.4,13X))

11110 I=KS1
11200 IF(I-1+100-KS2) 11201,11203,11203
11201 WRITE(3,136)
DO 11202 J=1,50
K=I+J
11202 WRITE(3,137)(E(K-1),SPECT2(K-1),E(K+49),SPECT2(K+49))
I=I+100
GO TO 11200
11203 WRITE(3,136)
LP=(KS2-I+1)/50
LC=(KS2-I+1)-50*LP
LD=LC+1
IF(LC)11204,11204,11205
11204 L=LP
LC=50
GO TO (1201,11224),L
11205 L=LP+1
GO TO (1201,1202),L
1201 DO 11211 J=1,LC
K=I+J
11211 WRITE(3,137)(E(K-1),SPECT2(K-1))
GO TO 206
1202 DO 11221 J=1,LC
K=I+J
11221 WRITE(3,137)(E(K-1),SPECT2(K-1),E(K+49),SPECT2(K+49))
11223 DO 11222 J=LD,50
K=I+J
11222 WRITE(3,137)(E(K-1),SPECT2(K-1))
GO TO 206
11224 DO 11225 J=LD,50
K=I+J
11225 WRITE(3,137)(E(K-1),SPECT2(K-1),E(K+49),SPECT2(K+49))
206 RETURN
END

```

C SUBROUTINE PRSCATT
 C PRSCATT PRINTS INFORMATION RELATED TO THE ATTENUATION DUE TO
 C SMALL-ANGLE MULTIPLE SCATTERING.....THE INFORMATION PRINTED AT
 C EACH POINT CONSISTS OF THE FOLLING.....ENERGY PER NUCLEON AT A
 C POINT,XBAR,SBAR,THETA, AND Y.
 C

```
COMMON ATTEN(500),SBAR(500),E(500),SIGMA(500),IND(500),LET(500),
2 N(500),SPECT2(50 ),THETAS(500),THETA(500),XBAR(500),Y(500),
3 XDATA(300),YDATA(300),F(500)
COMMON/GMDATA1/IMAX,DIFF,I8,PD
```

```
210 I=1
209 IF(I-IMAX)211,214,200
211 IF(I+49-IMAX)212,212,214
212 PRINT 130
      DO 213 J=1,50
        K=I+J
213 PRINT 131, E(K-1),XBAR(K-1),SBAR(K-1),THETA(K-1),Y(K-1),THETAS(K-1
2 )
      I=50+I
      GO TO 209
214 PRINT 130
      DO 215 J=I,IMAX
215 PRINT 131,E(J),XBAR(J),SBAR(J),THETA(J),      Y(J),THETAS(J)
130 FORMAT(1H1,8X,6HENERGY, 9X,11HPENETRATION,6X,16HMEAN DIST. TRAV- ,
2 5X,13HMEAN ANGLE OF,7X,      13HMEAN BEAM DE-/
3 5X,13H(MEV/NUCLEON),3X,18HDISTANCE (G/CM**2),3X,15HELLED (G/CM**
42) ,3X,16HDEFLECTION (RAD) ,4X,18HFLECTION (G/CM**2),3X,
5 6HTHETAS //)
131 FORMAT(6X,F9.3,8X,E11.4,9X,E11.4,8X,E11.4,9X,E11.4,5X,E11.4)
200 RETURN
      END
```



```
SUBROUTINE TABLE(XNAME)
  DIMENSION XNAME(15)
  ENDFILE 5
  REWIND 5
  CALL DATE(DTE)
  PRINT 200,DTE
200 FORMAT (1H1/100X,A10)
  PRINT 1,(XNAME(I),I=1,13)
  1 FORMAT(///13A10///1X,14HINITIAL ENERGY,4X,10HPEAK HALF-
  2 4X,12HPEAK/PLATEAU,4X,14HAVE. ENERGY AT,10X,4HMEAN,
  3 6X,8HDEPTH AT 5X,10HPERCENTAGE ,7X,9HMEAN BEAM/
  4 1X,13H(MEV/NUCLEON) ,7X,8HWIDTH
  5 5X,10HDOSE RATIO,4X,17HPEAK(MEV/NUCLEON),8X,5HRANGE,
  6 5X,9H PEAK ,3X,13HDETOUR FACTOR ,5X,10HDEFLECTION// )
  5 READ (5) E,WIDTH,TEMP1,EMEAN,X1,XBAR,DT,YMAX
  IF(ENDFILE 5)300,10
  10 PRINT 2,E,WIDTH,TEMP1,EMEAN,X1,XBAR,DT,YMAX
  2 FORMAT(4X,F7.2,7X,E10.3,5X,E11.4,6X,E11.4,8X,E11.4,2X,E10.3,
  2 4X,E11.4,5X,E10.3)
  GO TO 5
300 REWIND 5
  RETURN
  END
```

```

SUBROUTINE GMPRINT(KT)
REAL N ,LET
LOGICAL PLOTP,FRAME
COMMON ATTEN(500),SBAR(500),E(500),SIGMA(500),IND(500),LET(500),
2 N(500),SPECT2(500),THETAS(500),THETA(500),XBAR(500),Y(500),
3 XDATA(300),YDATA(300),F(500)
COMMON/GMDATA1/IMAX,DIFF,I8,PD
COMMON /GMDATA2/TITLE, FRAME,INNP,KS1,KS2
COMMON/DATA/NDTAPT,PLOTP
COMMON/CCPOOL/XMIN,XMAX,YMIN,YMAX,CCXMIN,CCXMAX,CCYMIN,CCYMAX
COMMON/CCFACT/FACTOR
EQUIVALENCE(TEM,Y),(STORE1,THETA)
DIMENSION TEM(500),STORE1(500)
DIMENSION YLABEL(13),XLABEL(13),YLABEL3(2),XLABEL2(3)
DIMENSION ROUND(10),XLABEL1(13),YLABEL1(2),YLABEL2(2),TITLE(15)
DATA (ROUND(I),I=1,4)/1.0,2.0,3.0,5.0/,NROUND/4/
DATA YLABEL1,YLABEL2/13HRELATIVE DOSE , 20HRELATIVE NUMBER FLUX/
DATA XLABEL1/30HPENETRATION DISTANCE (G/CM**2)/
DATA XLABEL2/24HENERGY (MEV PER NUCLEON) /
XLABEL(4)=10H
YLABEL(3)=10H
IF((.NOT.FRAME).AND.(INNP.GT.1))GO TO 9
FACTOR=100.0
CCXMIN=2.0
CCXMAX=11.0
CCYMIN=2.5
CCYMAX=8.88
PARTX=10.
NX1=10
PARTY=10.
NY1=10
KSIZE=2
9 IF(KT.EQ.0)GO TO 20
IF(KT.EQ.3)GO TO 35

```

C SET UP THE X- AND Y-ARRAYS AND AXIS LABELS

C SET UP FOR LET PRINTOUT

```

DO 30 I=1,IMAX
30 TEM(I)=LET(I)
DO 31 I=1,2
31 YLABEL(I)=YLABEL1(I)
DO 32 I=1,3
32 XLABEL(I)=XLABEL1(I)
NPT=IMAX
DO 33 I=1,NPT
33 STORE1(I)=XBAR(I)
GO TO 4

```

C SET UP FOR SPECTRUM PRINTOUT

```

35 NPT=KS2-KS1+1
DO 36 I=1,NPT
STORE1(I)=E(KS1+I-1)
36 TEM(I)=SPECT2(KS1+I-1)
DO 37 I=1,2
37 YLABEL(I)=YLABEL2(I)

```

```
DO 38 I=1,3
38 XLABEL(I)=XLABEL2(I)
GO TO 4
```

C SET UP FOR FLUX PRINTOUT

```
20 DO 21 I=1,IMAX
21 TEM(I)=N(I)
DO 22 I=1,2
22 YLABEL(I)=YLABEL2(I)
NPT=IMAX
DO 23 I=1,3
23 XLABEL(I)=XLABEL1(I)
DO 24 I=1,NPT
24 STORE1(I)=XBAR(I)
4 IF((.NOT.FRAME).AND.(INNP.GT.1))GO TO 11
```

C
C
C

SET UP DUMMY NUMBERS IN THE TWO ARRAYS FOR LINEUP

```
IF(PLOTP)GO TO 25
NDT=NPT
GO TO 80
25 DO 60 J=1,NDTAPT
TEM(NPT+J)=YDATA(J)
60 STORE1(NPT+J)=XDATA(J)
NDT=NPT+NDTAPT
```

C AXIS LABELS ADJUSTMENT

```
80 CALL LINEUP(STORE1,NDT,ROUND,NROUND,PARTX,XMIN,XMAX)
IF(XMIN.LE.0.0)GO TO 81
IF(KT.EQ.3)GO TO 70
81 NX1=NX1-INT(ABS(XMIN)*PARTX/(XMAX-XMIN)+1.0E-06)
3 XMIN=0.0
70 CALL LINEUP(TEM,NDT,ROUND,NROUND,PARTY,YMIN,YMAX)
IF(YMIN.EQ.0.0)GO TO 10
NY1=NY1-INT(ABS(YMIN)*PARTY/(YMAX-YMIN)+1.0E-06)
5 YMIN=0.0
```

C PLOT CURVE

```
10 CALL CCGRID(NX1,6HNOLBLS,NY1)
CALL FIXLBL(NX1,NY1,KSIZE,NXP,NYP)
KX=-NXP
KY=-NYP
IF(NXP.NE.0)GO TO 50
40 IF(NYP.NE.0)GO TO 51
GO TO 41
50 ENCODE(10,100,XLABEL(4))KX
100 FORMAT(7H X10** (12,1H))
GO TO 40
51 ENCODE(10,100,YLABEL(3))KY
GO TO 41
41 CALL CENTER(XLABEL,4,XLABEL,64)
CALL CENTER(YLABEL,3,YLABEL,46)
CALL CCLTR(2.1,9.08,0,3,TITLE,64)
CALL CCLTR(2.1,1.7,0,2,XLABEL,64)
CALL CCLTR(1.0,2.6,1,2,YLABEL,46)
```

```
11 CALL CCPLLOT(STORE1,TEM,NPT,4HJOIN)
   IF( PLOTP) CALL CCPLLOT(XDATA,YDATA,NDTAPT,6HNOJOIN,7,1)
   RETURN
   END
```

```
SUBROUTINE FIXLBL(NX1,NY1,KSIZE,NXP,NYP)
COMMON/CCPOOL/XMIN,XMAX,YMIN,YMAX,CCXMIN,CCXMAX,CCYMIN,CCYMAX
NFMT1=10H(F10.6)
NFMT2=10H(F10.7)
NFMT3=10H(F10.8)
CCXINT=(CCXMAX-CCXMIN)/NX1
CCYINT=(CCYMAX-CCYMIN)/NY1
XTEM=MAX1F(ABS(XMIN),ABS(XMAX))
YTEM=MAX1F(ABS(YMIN),ABS(YMAX))
ASSIGN 60 TO NNN1
ASSIGN 87 TO NNN2
XSTEP=1.0
YSTEP=1.0
DO 51 I=1,3
51 IF(CCXINT*XSTEP.LT.0.35*KSIZE)XSTEP=XSTEP+1.0
   IF(CCXINT*XSTEP.LT.0.35*KSIZE)ASSIGN 82 TO NNN1
   DO 52 I=1,3
52 IF(CCYINT*YSTEP.LT.0.1*KSIZE)YSTEP=YSTEP+1.0
   IF(CCYINT*YSTEP.LT.0.1*KSIZE)ASSIGN 100 TO NNN2
   GO TO NNN1
```

C X-AXIS NORMALIZATION AND LABELLING

```
60 NX=ALOG10(XTEM)+1.0E-10
   NXP=NX-1
   IF(NXP.GE.-2.AND.NXP.LT.1)GO TO 61
   XFCTR=10.0**({FLOAT(NXP)})
   GO TO 62
61 XFCTR=1.0
   NXP=0
62 XINT=ABS((XMAX-XMIN)/(NX1*XFCTR))
   XM=XMAX/XFCTR
   CCY=CCYMIN -KSIZE*0.10
   X=XMIN/XFCTR
   CCX=CCXMIN
70 AX=ABS(X)+1.0E-06
   IF(AX.GT.XM+1.0E-06)GO TO 82
   IF(AX.LT.0.001)GO TO 78
   IF(AX.GE.0.001.AND.AX.LT.1.0)GO TO 71
   IF(AX.GE.1.0.AND.AX.LT.10.0)GO TO 75
   IF(AX.GE.10.0.AND.AX.LT.100.0)GO TO 77
   GO TO 81
71 ENCODE(10,NFMT3,NTEMP)X
   XT=CCX-KSIZE*0.16
   GO TO 80
75 ENCODE(10,NFMT2,NTEMP)X
   XT=CCX-KSIZE*0.16
   GO TO 80
77 ENCODE(10,NFMT1,NTEMP)X
   XT=CCX-KSIZE*0.14
   GO TO 80
78 XT=CCX-KSIZE*0.02
   NTEMP=10H0
80 CALL CCLTR(XT,CCY,0,KSIZE,NTEMP,4)
81 CCX=CCX+CCXINT*XSTEP
   X=X+XINT*XSTEP
   GO TO 70
```

C Y-AXIS NORMALIZATION AND LABELLING

```
82 GO TO NNN2
87 NY=ALOG10(YTEM)+1.0E-10
  NYP=NY-1
  IF(NYP.GE.-2.AND.NYP.LT.1)GO TO 83
  YFCTR=10.0** (FLOAT(NYP))
  GO TO 84
83 YFCTR=1.0
  NYP=0
84 YINT=ABS((YMAX-YMIN)/(NY1*YFCTR))
  YM=YMAX/YFCTR
  CCX=CCXMIN -4*KSIZE*0.07
  CCY=CCYMIN-0.5*KSIZE*0.06
  Y=YMIN/YFCTR
85 AY=ABS(Y)+1.0E-06
  IF(AY.GT.YM+1.0E-06)GO TO 100
  IF(AY.LT.0.001)NTEMP=10H 0
  IF(AY.GE.0.001.AND.AY.LT.1.0)ENCODE(10,NFMT3,NTEMP)Y
  IF(AY.GE.1.0.AND.AY.LT.10.0)ENCODE(10,NFMT2,NTEMP)Y
  IF(AY.GE.10.0.AND.AY.LT.100.0)ENCODE(10,NFMT1,NTEMP)Y
  IF(Y.EQ.YMIN/YFCTR)CCY=CCY+0.03*KSIZE
  CALL CCLTR(CCX,CCY,0,KSIZE,NTEMP,4)
  IF(Y.EQ.YMIN/YFCTR)CCY=CCY-0.03*KSIZE
  CCY=CCY+CCYINT*YSTEP
  Y=Y+YINT*YSTEP
  GO TO 85
100 RETURN
  END
```

```

SUBROUTINE CENTER(NTEMP,N,NSAVE,M)
DIMENSION NFMT (5),NMASK(10),NTEMP(15)
DIMENSION NWORD(15),NSAVE(15),NHOLD(15),MASK(10)
DATA (NFMT (I),I=1,5)/1H(,1H ,2HX, ,1H ,4HA10) /,MASK1/1H /
DATA(NMASK(I),I=1,10)/00000055,000005500,000550000,055000000,
205500000000,05500 ,055000000000000,055000000000000000,
3055000000000000000 ,055000000000000000* /
DATA (MASK(I),I=1,10)/00000077,000007700,000770000,077000000,
207700000000,07700 ,077000000000000,07700000000000000,
3077000000000000000 ,0770000000000000000 /
IF(N.GT.13.OR.N.LT.1.OR.M.LT.1.OR.M.GT.132)RETURN
DO 110 I=1,N
110 NWORD(I)=NTEMP(I)
JM=N+1
DO 111 J=JM,15
111 NWORD(J)=MASK1
DO 100 J=1,15
100 NHOLD(J)=MASK1
NCOUNT=0
DO 10 I=1,N
IF(NWORD(I).NE.MASK1) GO TO 20
10 NCOUNT=NCOUNT+10
GO TO 239
20 DO 30 J=1,10
NCOMP=NWORD(I).AND.MASK(11-J)
IF(NCOMP.NE.NMASK(11-J)) GO TO 35
30 NCOUNT=NCOUNT+1
35 NSTORE=NCOUNT
DO 40 I=1,N
J=N+1-I
IF(NWORD(J).NE.MASK1) GO TO 45
40 NCOUNT=NCOUNT+10
45 DO 46 I=1,10
NCOMP=NWORD(J).AND.MASK(I)
IF(NCOMP.NE.NMASK(I)) GO TO 50
46 NCOUNT=NCOUNT+1
50 NCHAR=10*N-NCOUNT
IF(NCHAR.GT.112.OR.NCHAR.GT.M)RETURN
NBL=(M-NCHAR)/2
IM=NCHAR/10
IF(MOD(NCHAR,10).NE.0)IM=IM+1
IK=NSTORE+10*IM
IF(NSTORE.EQ.0)GO TO 210
ENCODE(10,70,NFMT(2))NSTORE
70 FORMAT(I10)
GO TO 220
210 NFMT(3)=10H
220 ENCODE(10,70 ,NFMT(4))IM
DECODE(IK,NFMT,NWORD)(NHOLD(I),I=1,IM)
DO 229 J=1,15
229 NWORD(J)=MASK1
NFMT(2)=1H)
IF(NBL.EQ.0)GO TO 54
IF(NBL.LT.10)GO TO 55
ENCODE(10,3,NFMT)NBL
3 FORMAT(1H(,I2,7HX,15A10)
GO TO 231
54 NFMT(1)=10H(15A10
GO TO 231
```

```
55 ENCODE(10,5,NFMT)NBL
5  FORMAT(1H(,I1,8HX,15A10 )
231 IM=IM+2
    IK=NBL+10*IM-MOD(NBL,10)+10
    IF(MOD(NBL,10).NE.0)IK=IK+10
    ENCODE(IK,NFMT,NWORD)(NHOLD(I),I=1,IM)
239 JM=M/10
    IF(MOD(M,10).NE.0)JM=JM+1
    DO 240 I=1,JM
240  NSAVE(I)=NWORD(I)
     NFMT(1)=1H(
     NFMT(2)=10H
     NFMT(3)=2HX,
     NFMT(4)=10H
     NFMT(5)=4HA10)
     RETURN
     END
```


REFERENCES

1. G. M. Litton, R. W. Wallace, and C. A. Tobias, Penetration of Heavy Ions in Matter, (unpublished).
2. R. D. Evans, The Atomic Nucleus (McGraw-Hill Book Co., New York, N. Y., 1955).
3. P. G. Steward and R. W. Wallace, Calculation of Stopping Power and Range-Energy Values for any Heavy Ion in Nongaseous Media, UCRL-17314, December 1966.
4. W. H. Barkas and M. J. Berger, Tables of Energy Losses and Ranges of Heavy Charged Particles, NAS-NRC 1133, 1964.
5. J. E. Turner, Values of I and IADJ ..., NAS-NRC 1133, 1964.
6. R. M. Sternheimer, Phys. Rev. 117, 485 (1960).

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

- A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

