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**U.S. DEPARTMENT OF COMMERCE**
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**Robert M. White, Under Secretary for Technology**

**NATIONAL INSTITUTE OF STANDARDS**
**AND TECHNOLOGY**
**John W. Lyons, Director**

# ESTAR, PSTAR and ASTAR: Computer Codes for Calculating Stopping-Power and Range Tables for Electrons, Protons, and Helium Ions

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This report describes three computer codes, ESTAR, PSTAR and ASTAR, which calculate stopping-power and range tables for electrons, protons, or helium ions, according to methods described in ICRU Reports 37 and 49. The codes provide output for electrons in any stopping material, and for protons and helium ions in 74 materials. Executable programs are provided which can be run on IBM-compatible personal computers. Fortran source code is also provided for implementing the codes on other computers.

*Contractor, work done under NIST contract 50SBNB9C555.

## 1. Introduction

Printed tables remain indispensable as a means of quickly looking up information, but there is an increasing need for computer-readable databases and for computer codes that can quickly generate the desired data. In order to meet such a need, this report presents computer programs ESTAR, PSTAR, and ASTAR which calculate stopping powers, ranges and related quantities, for electrons, protons and helium ions. The underlying methods were developed by a members of a report committee sponsored by the International Commission on Radiation Units and Measurements (ICRU).[1]

With a default option, ESTAR generates stopping powers and ranges for electrons which are the same as those tabulated in ICRU Report 37 (ICRU,1984) for 72 materials at a standard grid of 81 energies between 10 keV and 1000 MeV. ESTAR can also calculate similar tables for any other element, compound or mixture. Furthermore it can calculate stopping powers at any set of energies between 1 keV and 10 GeV.

With a default option, the PSTAR and ASTAR programs generate the stopping powers and ranges for protons and helium ions tabulated in ICRU Report 49 (ICRU, 1993) for 74 materials at a standard grid of 133 energies between 1 keV and 10 GeV for protons, and 122 energies between 1 keV and 1 GeV for helium ions. The codes can also calculate similar results at any other energy grid between these limits.

Executable codes are provided which can be used directly on IBM-compatible personal computers. In addition, Fortran source code and data files are included, which can be used to install the codes on different computers. Source code listings can be found in Appendix 2. All the files for ESTAR, PSTAR and ASTAR are supplied in three archive files named EST.EXE, PST.EXE and AST.EXE. These are self-extracting archive files. For example, all the files for ESTAR can be obtained by issuing the command EST.

## 2. ESTAR: Stopping Powers and Ranges for Electrons

### 2.1. *Output of ESTAR*

ESTAR calculates the following quantities:

a) Collision stopping power, MeV $cm^2/g$;
b) Radiative stopping power, MeV $cm^2/g$;
c) Total stopping power (sum of a and b), MeV $cm^2/g$;
d) Density effect parameter "delta";
e) CSDA range, $cm^2/g$;
f) Radiation yield (fraction of energy or primary electron converted into bremsstrahlung).

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[1]The members of this committee were H. H. Anderson, M. J. Berger (chairman), H. Bichsel, J. A. Dennis, M. Inokuti (vice-chairman), D. Powers, S. M. Seltzer, D. Thwaites, J. E. Turner, and D. E. Watt.

The significance of these quantities is briefly indicated in Appendix 1. Two output options are provided:

*Option 1*: A table is produced that includes all of the quantities a) through f) at a standard set energies between 10 keV and 1000 MeV. The spacing of the energy grid is approximately logarithmic. The output is a two-page table with a format similar to that used in ICRU Report 37.

*Option 2*: Output quantities a) through d) are tabulated at a user-selected set of energies between 1 keV and 10 GeV.

### 2.2. *Method*

Collision stopping powers are calculated from the theory of Bethe (1930,1932), with a density-effect correction evaluated according to Sternheimer (1952, 1982). The stopping-power formula contains an important parameter, the mean excitation energy (I-value), which characterizes the stopping properties of a material. I-values cannot be calculated accurately from first principles, but must be extracted from experimental data, mainly measured proton and alpha particles stopping powers and ranges, and also from oscillator-strength distributions for gases and dielectric response functions for materials in the condensed phase. In ESTAR, I-values are used that were adopted in ICRU Report 37 (ICRU, 1984). Other authors prefer slightly different I-values. Furthermore, the preferred choices can be expected to change in the course of time, as improved experimental information becomes available. Therefore the user of ESTAR is given the opportunity to replace the default I-values by different choices.

The uncertainties of the calculated collision stopping powers for electrons are estimated in (ICRU, 1984) to be 1 to 2 percent above 100 keV, 2 to 3 percent (in low-Z materials) and 5 to 10 percent (in high-Z materials) between 100 keV and 10 keV. The increasing uncertainties at low energies are due to the lack of shell corrections which are required when the velocity of the incident electron is no longer large compared to the velocities of the atomic electrons, especially those in the inner shells. Because of this limitation, tabulations of collision stopping powers are customarily restricted to energies above 10 keV. A similar restriction is recommended in regard to the use of the ESTAR.[2]

Radiative stopping powers are evaluated in ESTAR with a combination of theoretical bremsstrahlung cross sections described by Seltzer and Berger (1985). Analytical formulas (using a high-energy approximation) are used above 50 MeV, and accurate numerical results of Pratt *et al.* (1977) below 2 MeV. Cross sections in the intermediate energy region from 2 MeV to 50 MeV are obtained by interpolation, a procedure whose accuracy was confirmed by more detailed calculations for a few cases. The uncertainties of the radiative stopping powers are estimated to be 2 percent above 50 MeV, 2 to 5 percent between 50 and 2 MeV, and 5 percent below 2 MeV.

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[2]Due to the omission of shell corrections, the stopping powers from ESTAR are expected to be too large at very low energies. It is estimated that for materials of low atomic number, such as water, air or plastics, the error will be of the order of 10 percent at 1 keV. ESTAR will not run below 1 keV.

2.3. *Required Program and Data Files*

2.3.1. *Running ESTAR on IBM-compatible Personal Computers.* It is assumed that the operating system is DOS, Version 2.0 or higher. A mathematical coprocessor is required. The following files are used:

| | |
|---|---|
| ESTAR.EXE: | executable code |
| UEDAT: | atomic data, in an unformatted direct-access file |
| UCOMP: | data pertaining to the composition of materials, in an unformatted direct-access file |
| IDLIST.COM: | executable code that displays a list of material names included in the database UCOMP; |
| COMPOS.EXE: | executable code for examining the contents of the database UCOMP |
| ENG.ELE: | default energy list (81 values between 0.01 and 1000 MeV). |

2.3.2. *Installation of ESTAR on Different Computers.* The following additional files are supplied, consisting of Fortran-77 source code and data files in ASCII format:

| | |
|---|---|
| ESTAR.FOR: | Fortran source code |
| COMPOS.FOR: | Fortran source code |
| EDCONV.FOR: | ASCII-to-binary conversion program |
| CONVERT.FOR: | ASCII-to-binary conversion program |
| FEDAT: | Atomic data (formatted file) |
| FCOMP: | Data pertaining to the composition of materials (formatted file) |

These files are to be used as follows:

a) ESTAR.FOR, COMPOS.FOR, EDCONV.FOR and CONVERT.FOR must be compiled (and linked) to produce executable codes.
b) EDCONV must be run, using FEDAT as input. The output is an unformatted direct-access file UEDAT.
c) CONVERT must be run, using FCOMP as input. The output is the unformatted direct-access file UCOMP.

2.4. *How to Specify the Properties of the Stopping Medium*

ESTAR must be supplied with information about the atomic composition, the density, and the mean excitation energy (I-value) of the material. There are two ways in which this information can be provided:

*Option 1*: For 279 materials, the required information has been stored as a database in the file UCOMP which can be read by ESTAR. For these materials the user need merely specify the identification (ID) number of the material of interest.

*Option 2*: The information for any material can be supplied by the user from the keyboard, in response to prompts from ESTAR.

With both options, ESTAR provides a default I-value, which can be changed by the user.

2.4.1. *Use of the Database UCOMP.* UCOMP includes data for 279 materials, with ID numbers 1 to 278, and 906. Carbon appears twice, as amorphous carbon (ID = 6) and as graphite (ID = 906). ID numbers smaller than 99 pertain to elements, and are identical with atomic numbers. The others pertain to compounds or mixtures. Table 1 gives a listing of ID numbers and names of materials. Elements appear in order of increasing atomic number, and are followed by compounds and mixtures listed alphabetically. The user can use issue the command IDLIST to starts a program which lists, on the monitor screen, all ID numbers and material names in UCOMP. This display can be scrolled.

The contents of UCOMP for a specified ID number can be examined by running the program COMPOS. The program prompts the user to specify the desired material, in terms of the ID number. COMPOS then lists the atomic numbers and weights of the atomic constituents, the density of the material, and its I-value.

2.4.2. *Entry of Composition Data from the Keyboard.* With this option, the user is prompted to supply the following information:

a) Name of the material, to be used in table headings;
b) The density of the material, $g/cm^3$;
c) The classification of the material: element, compound or mixture;
d) The chemical symbol for the element, or the chemical formula for the compound, which must be entered in standard chemical notation, with upper and lower case letters; subscripts must be written on-line. For example, silicon is to be entered as Si, silicon dioxide as SiO2, and water as H2O.
e) For mixtures, the user must provide the number of constituents (which can be elements or compounds), the fractions by weight of these constituents, and their chemical symbols or formulas. If some of these constituents are included in the UCOMP data base, it is possible (but not required) to enter the information from the UCOMP file with the appropriate ID number. For example, for Pyrex glass (80.7% $SiO_2$, 12.9 % $B_2O_3$, 3.8% $Na_2O$, 2.2% $Al_2O_3$ and 0.4% $K_2O$ by weight), the input for $Al_2O_3$ and $SiO_2$ can be taken from UCOMP.

ESTAR calculates, and displays on the monitor, the fractions by weight of the atomic constituents in the mixture. The user is prompted to inspect these fractions, and can either accept them or enter different composition data.

With entry from the keyboard, the composition data are used by ESTAR to determine the I-value of the material. For compounds this is done by a modified Bragg-additivity rule described in ICRU (1984), with chemical binding and phase effects taken into account in an approximate manner. The use of this procedure results in I-values that for elements are the same, and for compounds are very close to those stored in UCOMP.

ESTAR provides the option of storing the composition data entered from the keyboard in a designated file, which can be merged into the FCOMP file. When an enlarged FCOMP file is used, the data statements KMAX/279/ in CONVERT.FOR and KLST/278/ in COMPOS.FOR must be appropriately changed.

2.5. *Energy List*

With Output Option 1 (as described in Section 2), an energy list need not be specified. With Output Option 2, there are three options for the energy-list input:

*Option 1*: A default list of energies is used from file ENG.ELE, consisting of 81 energies between 1 keV and 1000 MeV.

*Option 2*: A user-selected list of energies is used, that was previously stored by the user in a designated file. The first line of this file must contain the number of energies in the list, and subsequent lines must contain the energies (in MeV) separated by blanks.

*Option 3*: The desired list of energies may be entered from the keyboard, as prompted by ESTAR.

With Options 2 and 3, ESTAR issues a warning if at least one of the energies is smaller than 10 keV, and halts if an energy is below 1 keV.

## 3. PSTAR and ASTAR Programs for Protons and Helium Ions

3.1. *Output of PSTAR and ASTAR*

The following quantities are calculated:

a) Electronic (collision) stopping power, MeV $cm^2/g$;
b) Nuclear stopping power, MeV $cm^2/g$;
c) Total stopping power (sum of a and b), MeV $cm^2/g$;
d) CSDA range, $g/cm^2$;
e) Projected range, $g/cm^2$;
f) Detour factor (ratio of projected range to CSDA range).

The significance of these quantities is indicated in Appendix 1.

3.2. *Required Program and Data Files*

3.2.1. *Running PSTAR or ASTAR on an IBM-compatible Personal Computer.* It is assumed that the operating system is DOS, Version 2.0 or higher. A mathematical coprocessor is required. The following files are used to run PSTAR:

| | |
|---|---|
| PSTAR.EXE: | executable code for generating a stopping-power and range table |
| UPROT: | database that contains stopping power and range data |
| MATS: | set of names of 74 materials in the database |
| ENG.PRO: | default energy list (133 energies between 1 keV and 10,000 MeV) |
| UCOMP: | file that contains material composition data |
| COMPOS.EXE: | executable code for examining the contents of UCOMP |
| IDL.COM: | executable code that displays a list of material names and corresponding ID numbers; |

The following files are used to run ASTAR:

| | |
|---|---|
| ASTAR.EXE: | executable code for generating a stopping-power and range table |
| UALPH: | database that contains stopping power and range data |
| MATS: | set of names of 74 materials in the database |
| ENG.ALF: | default energy list (122 energies between 1 keV and 1000 MeV) |
| UCOMP: | file that contains information about the composition of the materials included in the database; |
| COMPOS.EXE: | executable code for examining the contents of UCOMP for a specified material; |
| IDL.COM: | executable code that displays a list of material names and corresponding ID numbers. |

3.2.2. *Installation of PSTAR or A STAR on Different Computers*. The following additional files are supplied, consisting of Fortran-77 source code and data files in ASCII format:

| For Protons | For Helium Ions | For Both |
|---|---|---|
| PSTAR.FOR | ASTAR.FOR | COMPOS.FOR |
| PCONV.FOR | ACONV.FOR | CONVERT.FOR |
| FPROT | FALPH | FCOMP |

Source-code listings can be found in Appendix 2. These files are to be used as follows:

a) PSTAR.FOR or ASTAR.FOR must be compiled (and linked) to produce executable codes.
b) PCONV.FOR must be compiled and run, using the formatted file FPROT as input. The output is the unformatted direct-access file UPROT.
c) ACONV.FOR must be compiled and run, using the formatted file FALPH as input. The output is the unformatted direct-access file UALPH.
d) CONVERT.FOR must be compiled and run, using the formatted file FCOMP as input. The output is the unformatted direct-access binary file UCOMP.
e) COMPOS.FOR must be compiled, and can be used to examine the contents of the UCOMP file.

3.3. *List of Materials*

For easy reference in the computer programs, each material is given an identification (ID) number. For elements the ID numbers are identical with atomic numbers (except for graphite which has ID number 906, to distinguish it from amorphous carbon with ID number 6).

Table 1 list the names and ID numbers of the 74 materials in the data files. The list includes 26 elements and 48 compounds and mixtures. A listing of ID numbers and names can also be displayed, and scrolled, on the monitor screen by running the program IDL.

The information in the composition file UCOMP for each material consists of:

a) The atomic numbers and fractions by weight of the constituent atoms;
b) The density;
c) The mean excitation energy of the material, which is a key parameter in Bethe's stopping power formula.

The contents of UCOMP for a material of interest can be stored on a designated file by running the program COMPOS.

### 3.4. *List of Energies*

There are three options for selecting energies. Note that energies must not be smaller than 0.001 MeV, or greater than 10000 MeV for protons or 1000 MeV for helium ions.

*Option 1*: A default list of energies is used, stored in file ENG.PRO for protons (133 energies between 1 keV and 10000 MeV) or in ENG.ALF for helium ions (122 energies between 1 keV and 1000 MeV).

*Option 2*: A user-selected list of energies is used, assuming that it was previously stored in a designated file. The first line of this file must contain the number of energies in the list, and subsequent lines must contain the energies (in MeV) separated by blanks.

*Option 3*: The desired list of energies may be entered from the keyboard, as prompted by the PSTAR or ASTAR program.

### 3.5. *Methods Used To Evaluate of Stopping Powers*

Only a brief indication of the methods used for protons and helium ions is given here. For details, the reader is referred to the forthcoming ICRU Report 49 (ICRU, 1993). At high energies, collision stopping powers are evaluated using Bethe's stopping-power formula (Bethe, 1930). At low energies, fitting-formulas are used which are based on experimental stopping power data. The boundary between the high- and low-energy regions was at approximately 0.5 MeV for protons, and 2 MeV for alpha particles.

For each material, the experimental stopping powers at energies below a cut-off energy $T_1$, together with the theoretical values from the Bethe theory at energies above a cut-off energy $T_2$, are fitted by single cubic spline. Typical values are $T_1 = 0.2$ MeV for protons and 1.0 MeV for helium ions, and $T_2 = 0.5$ MeV for protons and 2.0 MeV for helium ions. This spline function is used for interpolation at energies between $T_1$ and $T_2$. The two cut-off energies are adjusted individually for each material to obtain a visually pleasing plot of stopping power *vs.* energy.

In ICRU (1992) the uncertainties of the collision stopping powers in the high-energy region are stated to be 1 to 2 percent for elements, and 1 to 4 percent for compounds. The uncertainties are more difficult to estimate in the low-energy region. In ICRU (1992) they are estimated to be 2 to 5 percent at 1000 keV, 5 to 10 percent at 100 keV, 10 to 15 percent at 10 keV, and at least 20 to 30 percent at 1 keV.

3.5.1. *Stopping Power Theory at High Energies.* The stopping power formula used in the high-energy region included various correction terms: (a) shell corrections, which are important when the proton velocity is not large compared to the velocities of the atomic electrons; (b) the Barkas and Bloch corrections, which take into account departures from the first-order Born approximation; and (c) the density-effect correction, which is noticeable only for protons with energies above several hundred MeV.

The values of the mean excitation energies used in the stopping power formula are the same as those adopted in ICRU Report 37 (ICRU, 1984). They are based on the analysis of measured stopping powers, and on information extracted from empirical oscillator strengths and dielectric response functions. For compounds, the mean excitation energies take into account, by a crude approximation, differences between the gaseous and condensed phase, and the effects of chemical binding.

The shell corrections for most elements are based on semi-empirical formulas developed by Bichsel and described in ICRU (1984). For elements with atomic numbers $Z > 63$, and for $Z = 47$, revised shell corrections from Bichsel (1991) are used. The Bloch correction is evaluated from the formula given by Bloch (1933). The Barkas correction is calculated according to the method of Ashley, Ritchie and Brandt (1972,1973), with parameter values recommended by Bichsel (ICRU,1984). For elements with atomic numbers $Z \geq 64$, and for $Z = 47$, empirical formulas of Bichsel (1990) are used for the Barkas correction.

3.5.2. *Empirical Stopping Powers at Low Energies.* In the low-energy region, stopping powers are calculated from fitting formulas that represent experimental data for many elements and a limited number of compounds. Extensive use is made of a fitting formula of Varelas and Biersack (1970), with numerical coefficients adopted in ICRU (1992), which - except for a few materials - are from Andersen and Ziegler (1977) for protons, and from Ziegler (1977) or Watt (1988) for alpha particles. For elements without experimental data, stopping powers were obtained by Andersen and Ziegler (1977) and by Ziegler (1977) through interpolation with respect to atomic number, and were then fitted by the Varelas-Biersack formula. For a few materials a different fitting formula for alpha-particle stopping powers developed by Powers (1978) was used.

For compounds for which no experimental stopping power data are available, the Bragg additivity rule was used, and mass stopping powers were calculated as linear combinations of the mass stopping powers of the constituents atoms. When applying the additivity rule to mixtures, these are treated, to the extent possible, as a mixtures of compounds and elements. For example, the stopping power of "muscle" is obtained by as a weighted sum of the stopping power of water (assumed to be 78.6% by weight) and the stopping powers of the other elemental constituents.

3.5.3. *Nuclear Stopping Powers.* Cross sections for the elastic scattering of charged particles by atoms are obtained by a classical-mechanics orbit calculation, using the method of Everhart, Stone and Carbone (1955). For protons the screened potential is assumed to be the Thomas-Fermi potential as parameterized by Moliere (1947). For alpha particles, the "universal" ion-atom potential of Ziegler, Biersack and Littmark (1985) is used. Nuclear stopping powers are calculated using the relation between the deflection angles and the energy transfers to the recoiling atom in elastic collisions. In ICRU (1992) the uncertainties of nuclear stopping powers for alpha particles are estimated to be 5 to 10 percent at 100 keV, 10 percent at 10 keV, and 10 to 20 percent at 1 keV.

3.5.4. *CSDA and Projected Ranges.*

CSDA ranges are calculated in the continuous-slowing-down approximation by integrating the reciprocal of the total stopping power (collision plus nuclear) with respect to energy. Projected ranges are obtained in a transport calculation according to the method of Lewis (1950), which uses the elastic scattering cross sections discussed in Section 3.5.3.

## Appendix 1: Significance of Calculated Quantities

*Collision stopping power*: average rate of energy loss per unit path length, due to Coulomb collisions that result in the ionization and excitation of atoms. For heavy charged particles, the collision stopping power is often called *electronic stopping power*.

*Density-effect correction*: enters into the formula for the collision stopping power and takes into account the reduction of the collision stopping power due to the polarization of the medium by the incident electron.

*Radiative stopping power*: average rate of energy loss per unit path length due to collisions with atoms and atomic electrons in which bremsstrahlung quanta are emitted. Important only for electrons.

*Nuclear stopping power*: average rate of energy loss per unit path length due to the transfer of energy to recoiling atoms in elastic collisions. Important only for heavy charged particles.

*Total stopping power*: for electrons, the sum of the collision and radiative stopping powers; for protons and helium ions, the sum of collision and nuclear stopping powers.

*CSDA range*: a very close approximation to the average path length traveled by a charged particle as it slows down to rest, calculated in the continuous-slowing-down approximation. In this approximation, the rate of energy loss at every point along the track is assumed to be equal to the same as the total stopping power. Energy-loss fluctuations are neglected. The CSDA range is obtained by integrating the reciprocal of the total stopping power with respect to energy.

*Projected range*: average value of the depth to which a charged particle will penetrate in the course of slowing down to rest. This depth is measured along the initial direction of the particle.

*Detour factor*: ratio of the projected range to the CSDA range. As the result of multiple scattering, the trajectory of the particle is wiggly rather than straight, and the detour factor is always smaller than unity.

*Radiation yield*: average fraction of the initial kinetic energy of an electron that is converted to bremsstrahlung energy as a particle slows down to rest, calculated in the continuous-slowing-down approximation. Important only for electrons.

# Appendix 2: Program Listing

```
      PROGRAM ESTAR
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION ATB(100),MZ(14),WT(14),G(14),AT(14),NC(26),BD(26),
     1 T(1001),TL(1001),CLOSS(1001),RLOSS(1001),RLOSSL(1001),
     2 TLOSS(1001),TLOSSL(1001),AST(1001),BST(1001),CST(1001),DST(1001),
     4 ART(1001),BRT(1001),CRT(1001),DRT(1001),DLT(1001),ER(113),
     5 ERL(113),RLOS(113),RLOST(113),RLOSTL(113),ARL(113),BRL(113),
     6 CRL(113),DRL(113),ALF(1000),EPS(1000),EN(1000),F(1000),Q(1200),
     7 YQ(1200),YQL(1200),D(1200),ADEL(1200),BDEL(1200),CDEL(1200),
     8 DDEL(1200),GRAND(81),GRAND1(81),RG(113),RAD(113)
      CHARACTER ENGIN*30,MAT*72,FF*1,OUTPUT*30,
     1 DATFIL*30,MEAD1*13,BL*61,MEAD2*120,MEAD3*120
      DATA ATB/
     1 1.00794D0,4.002602D0,6.941D0,9.012182D0,10.811D0,12.011D0,
     2 14.00674D0,15.9994D0,18.9984032D0,20.1797D0,22.989768D0,
     3 24.3050D0,26.981539D0,28.0855D0,30.973762D0,32.066D0,35.4527D0,
     4 39.948D0,39.0983D0,40.078D0,44.955910D0,47.88D0,50.9415D0,
     5 51.9961D0,54.93805D0,55.847D0,58.93320D0,58.69D0,63.546D0,
     6 65.39D0,69.723D0,72.61D0,74.92159D0,78.96D0,79.904D0,83.80D0,
     7 85.4678D0,87.62D0,88.90585D0,91.224D0,92.90638D0,95.94D0,
     8 97.9072D0,101.07D0,102.9055D0,106.42D0,107.8682D0,112.411D0,
     9 114.82D0,118.710D0,121.75D0,127.60D0,126.90447D0,131.29D0,
     1 132.90543D0,137.327D0,138.9055D0,140.115D0,140.90765D0,144.24D0,
     2 144.9127D0,150.36D0,151.965D0,157.25D0,158.92534D0,162.50D0,
     3 164.93032D0,167.26D0,168.93421D0,173.04D0,174.967D0,178.49D0,
     4 180.9479D0,183.85D0,186.207D0,190.2D0,192.22D0,195.08D0,
     5 196.96654D0,200.59D0,204.3833D0,207.2D0,208.98037D0,208.9824D0,
     6 209.9871D0,222.0176D0,223.0197D0,226.0254D0,227.0278D0,
     7 232.0381D0,231.03588D0,238.0289D0,237.0482D0,239.0522D0,
     8 243.0614D0,247.0703D0,247.0703D0,251.0796D0,252.083D0,
     9 257.0951D0/
      DATA LKMAX/113/
      DATA ER/1.00E-03,1.25E-03,1.50E-03,1.75E-03,2.00E-03,2.50E-03,
     1        3.00E-03,3.50E-03,4.00E-03,4.50E-03,5.00E-03,5.50E-03,
     2        6.00E-03,7.00E-03,8.00E-03,9.00E-03,1.00E-02,1.25E-02,
     3        1.50E-02,1.75E-02,2.00E-02,2.50E-02,3.00E-02,3.50E-02,
     4        4.00E-02,4.50E-02,5.00E-02,5.50E-02,6.00E-02,7.00E-02,
     5        8.00E-02,9.00E-02,1.00E-01,1.25E-01,1.50E-01,1.75E-01,
     6        2.00E-01,2.50E-01,3.00E-01,3.50E-01,4.00E-01,4.50E-01,
     7        5.00E-01,5.50E-01,6.00E-01,7.00E-01,8.00E-01,9.00E-01,
     8        1.00E+00,1.25E+00,1.50E+00,1.75E+00,2.00E+00,2.50E+00,
     9        3.00E+00,3.50E+00,4.00E+00,4.50E+00,5.00E+00,5.50E+00,
     1        6.00E+00,7.00E+00,8.00E+00,9.00E+00,1.00E+01,1.25E+01,
     2        1.50E+01,1.75E+01,2.00E+01,2.50E+01,3.00E+01,3.50E+01,
     3        4.00E+01,4.50E+01,5.00E+01,5.50E+01,6.00E+01,7.00E+01,
     4        8.00E+01,9.00E+01,1.00E+02,1.25E+02,1.50E+02,1.75E+02,
     5        2.00E+02,2.50E+02,3.00E+02,3.50E+02,4.00E+02,4.50E+02,
     6        5.00E+02,5.50E+02,6.00E+02,7.00E+02,8.00E+02,9.00E+02,
     7        1.00E+03,1.25E+03,1.50E+03,1.75E+03,2.00E+03,2.50E+03,
     8        3.00E+03,3.50E+03,4.00E+03,4.50E+03,5.00E+03,5.50E+03,
     9        6.00E+03,7.00E+03,8.00E+03,9.00E+03,1.00E+04/
      DATA QBEG/1.0D-04/,NUMQ/50/,LMAX/1101/,MDAUX/0/,ISTORE/2/
      DATA COFF/0.307072D0/,RMASS/0.510999906D0/,MGRD/21/
      DATA LP/73/
    1 FORMAT(1H )
    5 FORMAT(A)
      OPEN (3,'UEDAT',FORM='UNFORMATTED',ACCESS='DIRECT',RECL=1224)
      OPEN (4,'UCOMP',FORM='UNFORMATTED',ACCESS='DIRECT',RECL=268)
      BL='                                                            '
      FF=CHAR(12)
      PRINT *,' Output options: '
      PRINT *,'    1) Stopping powers, ranges and radiation yields,'
      PRINT *,'       for standard energy grid'
      PRINT *,'    2) Stopping powers only,'
      PRINT *,'       for user-selected energy grid'
      PRINT *,' Choose 1 or 2: '
      READ *, MOUT
      PRINT *,' Options for entering properties of stopping material:'
      PRINT *,'    1) Use input from composition file UCOMP'
      PRINT *,'    2) Enter composition data from keyboard, as prompted'
      PRINT *,' Choose 1 or 2: '
      READ *, INMAT
      GO TO (15,10), INMAT
   10 CALL CPREP (MAT,KMAT,POT,RHO,MMAX,MZ,WT,ISTORE,DATFIL)
      POTL=LOG(POT*1.0D-06)
      GO TO 35
   15 PRINT *,' Enter ID number of material: '
      READ *, JPIC
      IF(JPIC-278)20,20,16
   16 IF(JPIC-906)18,17,18
   17 JPIC=279
      GO TO 20
   18 PRINT 19, JPIC
   19 FORMAT(I6,' is not an allowed ID number.')
      STOP 1
   20 READ (4,REC=JPIC) MAT,MMAX,ZAG,POT,RHO,MZ,WT
      PRINT 25,POT
   25 FORMAT(' I-value from UCOMP file is = ',F6.1,' eV.')
      PRINT *, ' Is this value acceptable (1=yes,2=no): '
      READ *, IPOT
      IF(IPOT.EQ.1) GO TO 30
      PRINT *,' Enter desired I-value (eV): '
      READ *, POT
   30 POTL=LOG(POT*1.0E-06)
   35 IF(MOUT.EQ.1) GO TO 80
      PRINT *,' Options for entering energy list:'
      PRINT *,'    1) Use default file ENG.ELE'
      PRINT *,'    2) Use prepared file'
      PRINT *,'    3) Entry from keyboard'
      PRINT *,' Choose 1, 2, or 3: '
      READ *, INEN
      GO TO (40,50,70), INEN
   40 ENGIN='ENG.ELE'
      GO TO 55
   50 PRINT *,' Enter name of energy-list file: '
      READ 5, ENGIN
   55 OPEN (7,FILE=ENGIN)
      READ (7,*) IMAX
      READ (7,*) (T(I),I=1,IMAX)
      CLOSE (7)
   60 TMIN=1.0E12
      DO 61 I=1,IMAX
      IF(T(I).LT.TMIN) TMIN=T(I)
   61 CONTINUE
      IF(TMIN-0.001D0)62,64,64
   62 PRINT 63
   63 FORMAT(' At least one of the specified energies is below 0.001 MeV
     1, out or range.')
      STOP
   64 IF(TMIN-0.01D0)65,80,80
   65 PRINT 66
   66 FORMAT('  Warning: at energies below 0.01 MeV, accuracy of')
      PRINT 67
   67 FORMAT('           collision stopping may be poor.')
      PAUSE
      GO TO 80
   70 PRINT *,' Specify the number of energies in the list: '
      READ *, IMAX
      PRINT *,' Enter all energies (in MeV): '
      READ *,(T(I),I=1,IMAX)
      GO TO 60
   80 PRINT *,' Enter name of output file: '
      READ 5, OUTPUT
      OPEN (UNIT=8,FILE=OUTPUT)
      QFAC=10.0D0**(1.0D0/DBLE(NUMQ))
      Q(1)=QBEG
      DO 90 L=2,LMAX
   90 Q(L)=Q(L-1)*QFAC
      DO 100 LK=1,LKMAX
  100 ERL(LK)=LOG(ER(LK))
      IF(MOUT.EQ.2) GO TO 106
      IMAX=LKMAX
      DO 105 I=1,IMAX
      T(I)=ER(I)
  105 TL(I)=ERL(I)
  106 GTOT=0.0
      DO 110 M=1,MMAX
      JZ=MZ(M)
      AT(M)=ATB(JZ)
      Z=DBLE(MZ(M))
      A=AT(M)
      G(M)=WT(M)*Z/A
  110 GTOT=GTOT+G(M)
      ZAV=GTOT
      HOM=28.81593D0*SQRT(RHO*ZAV)
      PMIL=2.0D0*LOG(POT/HOM)
      CBAR=PMIL+1.0D0
      DO 120 M=1,MMAX
  120 G(M)=G(M)/GTOT
      NBAS=0
      DO 130 LK=1,LKMAX
  130 RLOST(LK)=0.0
      DO 200 M=1,MMAX
      IZ=MZ(M)
      READ (3,REC=IZ) NMAX,LKIN,NC,BD,RLOS
      IF(LKIN.NE.LKMAX) STOP 2
      DO 140 LK=1,LKMAX
  140 RLOST(LK)=RLOST(LK)+WT(M)*RLOS(LK)
      IF(NC(NMAX))150,170,170
  150 NC(NMAX)=-NC(NMAX)
      IF(MMAX-1)160,160,170
  160 BD(NMAX)=0.0
  170 NSUM=0
      DO 180 N=1,NMAX
  180 NSUM=NSUM+NC(N)
      SUM=DBLE(NSUM)
      DO 190 N=1,NMAX
      NN=N+NBAS
      F(NN)=NC(N)*G(M)/SUM
  190 EN(NN)=BD(N)
  200 NBAS=NBAS+NMAX
      DO 210 LK=1,LKMAX
  210 RLOSTL(LK)=LOG(RLOST(LK))
      CALL SCOF(ERL,RLOSTL,LKMAX,ARL,BRL,CRL,DRL)
      NMAX=NBAS
```

```
      DO 390 N=1,NMAX
  390 ALF(N)=2.0/3.0
      IF(EN(NMAX))400,400,410
  400 ALF(NMAX)=1.0
  410 DO 420 N=1,NMAX
  420 EPS(N)=(EN(N)/MOM)**2
      ROOT=1.0
  430 FUN=-PHIL
      DER=0.0
      DO 440 N=1,NMAX
      TRH=ROOT*EPS(N)+ALF(N)*F(N)
      FUN=FUN+F(N)*LOG(TRH)
  440 DER=DER+F(N)*EPS(N)/TRH
      DROOT=FUN/DER
      ROOT=ROOT-DROOT
      IF(ABS(DROOT)-0.00001)450,450,430
  450 FACTOR=SQRT(ROOT)
      DO 460 N=1,NMAX
  460 EPS(N)=ROOT*EPS(N)
      IF(EN(NMAX))470,470,480
  470 YCUT=0.0
      GO TO 500
  480 SUM=0.0
      DO 490 N=1,NMAX
  490 SUM=SUM+F(N)/EPS(N)
      YCUT=1.0/SUM
  500 DO 530 L=1,LMAX
      SUM=0.0
      DO 510 N=1,NMAX
  510 SUM=SUM+F(N)/(EPS(N)+Q(L))
      YQ(L)=1.0/SUM
      YQL(L)=LOG(YQ(L))
      SUM=0.0
      DO 520 N=1,NMAX
      ARG=1.0+Q(L)/(EPS(N)+ALF(N)*F(N))
  520 SUM=SUM+F(N)*LOG(ARG)
      D(L)=SUM-Q(L)/(YQ(L)+1.0)
  530 CONTINUE
      TCUT=RMASS*(SQRT(YCUT+1.0)-1.0)
      IF(MDAUX.EQ.0) GO TO 560
      OPEN (UNIT=10,FILE='DAUX')
      WRITE (10,540)
  540 FORMAT(9X,'ZAV',9X,'RHO',9X,'MOM',9X,'POT',6X,'FACTOR',
     1 8X,'CBAR',8X,'TCUT',2X,'HMAX',2X,'NMAX')
      WRITE (10,545) ZAV,RHO,MOM,POT,FACTOR,CBAR,TCUT,HMAX,NMAX
  545 FORMAT(7F12.6,2I6)
      WRITE (10,1)
      WRITE (10,550) (YQ(L),L=1,LMAX,10)
      WRITE (10,550) (D(L),L=1,LMAX,10)
  550 FORMAT(1P4E17.9)
      CLOSE (10)
  560 CALL SCOF(YQL,D,LMAX,ADEL,BDEL,CDEL,DDEL)
      DO 595 I=1,IMAX
      E=T(I)
      TAU=T(I)/RMASS
      Y=TAU*(TAU+2.0)
      BETQ=Y/((TAU+1.0)**2)
      DELTA=0.0D0
      IF(Y.LT.YQ(1)) GO TO 590
      IF(Y.LE.YCUT) GO TO 590
      IF(Y-YQ(LMAX))585,585,580
  580 PRINT *,' YQ(LMAX) out of range'
      STOP 3
  585 YL=LOG(Y)
      CALL BSPOL(YL,YQL,ADEL,BDEL,CDEL,DDEL,LMAX,DELTA)
  590 DENCOR=0.5D0*DELTA
      DLT(I)=DELTA
      SPART=LOG(T(I))-POTL+0.5*LOG(1.0+0.5*TAU)-DENCOR
      TERM=(1.0-BETQ)*(1.0+(TAU**2)/8.0-(2.0*TAU+1.0)*LOG(2.0))
      STNUM=SPART+0.5*TERM
      CLOSS(I)=COFF*ZAV*STNUM/BETQ
      EL=LOG(E)
      CALL BSPOL(EL,ERL,ARL,BRL,CRL,DRL,LKMAX,RES)
      RLOSS(I)=EXP(RES)
      TLOSS(I)=CLOSS(I)+RLOSS(I)
  595 CONTINUE
      IF(MOUT.EQ.2) GO TO 700
      DO 600 I=1,IMAX
      RLOSSL(I)=LOG(RLOSS(I))
  600 TLOSSL(I)=LOG(TLOSS(I))
      CALL SCOF(TL,TLOSSL,IMAX,AST,BST,CST,DST)
      CALL SCOF(TL,RLOSSL,IMAX,ART,BRT,CRT,DRT)
      RG(1)=0.5D0*T(1)/TLOSS(1)
      RAD(1)=0.5D0*T(1)*RLOSS(1)/TLOSS(1)
      DO 690 I=2,IMAX
      ETMAX=T(I)
      ETMIN=T(I-1)
      EDIFF=(ETMAX-ETMIN)/DBLE(MGRD-1)
      DET=EDIFF/3.0D0
      DO 685 M=1,MGRD
      ETL=LOG(ETMAX-EDIFF*DBLE(M-1))
      CALL BSPOL(ETL,TL,AST,BST,CST,DST,IMAX,RES)
      GRAND(M)=1.0D0*EXP(-RES)
      CALL BSPOL(ETL,TL,ART,BRT,CRT,DRT,IMAX,RESR)
  685 GRAND1(M)=EXP(RESR)*GRAND(M)
      CALL GRAL(DET,GRAND,MGRD,STEP)
      CALL GRAL(DET,GRAND1,MGRD,DRAD)
      RG(I)=RG(I-1)+STEP
      RAD(I)=RAD(I-1)+DRAD
  690 CONTINUE
      DO 695 I=1,IMAX
  695 RAD(I)=RAD(I)/T(I)
      GO TO 790
  700 WRITE (8,705) MAT
  705 FORMAT(6X,'Electrons in ',A)
      WRITE (8,1)
      WRITE (8,706)
  706 FORMAT(9X,'Z/A',2X,'Density, g/cm3',4X,'I, eV')
      WRITE (8,707) ZAG,RHO,POT
  707 FORMAT(0PF12.6,1PE16.4,0PF9.1)
      WRITE (8,1)
      WRITE (8,710)
  710 FORMAT('      T = kinetic energy, MeV')
      WRITE (8,720)
  720 FORMAT(' CLOSS = collision stopping power, MeV cm2/g')
      WRITE (8,730)
  730 FORMAT(' RLOSS = radiative stopping power, MeV cm2/g')
      WRITE (8,740)
  740 FORMAT(' TLOSS = total stopping power, MeV cm2/g')
      WRITE (8,750)
  750 FORMAT(' DELTA = density effect parameter delta')
      WRITE (8,1)
      WRITE (8,760)
  760 FORMAT(11X,'T',7X,'CLOSS',7X,'RLOSS',7X,'TLOSS',7X,'DELTA')
      DO 780 I=1,IMAX
      WRITE (8,770) T(I),CLOSS(I),RLOSS(I),TLOSS(I),DLT(I)
  770 FORMAT(1PE12.4,1P3E12.4,0PF12.5)
  780 CONTINUE
      GO TO 875
  790 HEAD1='Electrons in '
      HEAD2=HEAD1//MAT
      DO 791 L=120,1,-1
      IF(HEAD2(L:L).NE.' ') GO TO 792
  791 CONTINUE
  792 LENGTH=L
      LSHIFT=6+(LP-LENGTH)/2
      HEAD3=BL(1:LSHIFT)//HEAD2
      WRITE (8,5) HEAD3
      WRITE (8,1)
      WRITE (8,793)
  793 FORMAT(30X,'Density, g/cm3',5x,'I, eV')
      WRITE (8,794) RHO,POT
  794 FORMAT(30X,1PE12.4,0PF12.1)
      WRITE (8,1)
      WRITE (8,1)
      WRITE (8,1)
      WRITE (8,800)
  800 FORMAT ( 2X,'    ENERGY          STOPPING POWER              CSDA
     1   RADIATION   DENSITY')
      WRITE (8,810)
  810 FORMAT ( 2X,'             COLLISION  RADIATIVE    TOTAL      RANGE
     1     YIELD      EFFECT')
      WRITE (8,820)
  820 FORMAT ( 2X,'
     1               DELTA')
      WRITE (8,830)
  830 FORMAT ( 2X,'     MeV    MeV cm2/g  MeV cm2/g  MeV cm2/g    g/cm2'
     1)
      DO 855 I=17,56
      IF (REAL((I-1)/8).NE.REAL(I-1)/8.0) GO TO 840
      WRITE (8,1)
  840 WRITE (8,850) T(I),CLOSS(I),RLOSS(I),TLOSS(I),RG(I),RAD(I),DLT(I)
  850 FORMAT (2X,0PF10.4,1P6E11.3)
  855 CONTINUE
      WRITE (8,5) FF
      WRITE (8,5) HEAD3
      WRITE (8,1)
      WRITE (8,793)
      WRITE (8,794) RHO,POT
      WRITE (8,1)
      WRITE (8,1)
      WRITE (8,1)
      WRITE (8,800)
      WRITE (8,810)
      WRITE (8,820)
      WRITE (8,830)
      DO 870 I=57,97
      IF (REAL((I-1)/8).NE.REAL(I-1)/8.0) GO TO 860
      WRITE (8,1)
  860 WRITE (8,850) T(I),CLOSS(I),RLOSS(I),TLOSS(I),RG(I),RAD(I),DLT(I)
  870 CONTINUE
  875 CLOSE (8)
      GO TO (880,900), ISTORE
  880 PRINT 890, DATFIL
  890 FORMAT('  Composition file ',A)
      PRINT *,' has been generated.'
  900 STOP
      END

      SUBROUTINE CPREP (MAT,KMAT,POT,RHO,MMAX,JZ,WT,ISTOR,OUTFIL)
C     30 Jul 89. Prepares input data for compound or mixture.
C                Derived in part from SPEC in XCOM, 2 Apr 87.
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      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION JZ(14),WT(140),JZ1(14),WT1(14),LH(100),WATE(100),
     1 FRAC(100),JZIP(100),ZAV1(14),POT1(14)
      CHARACTER FORMLA*72,FRM(100)*30,MAT*72,MAT1*72,
     1 OUTFIL*30,IDNO*3
      DATA RHOCUT/0.1/
    1 FORMAT(1H )
    5 FORMAT(A)
      PRINT *,' Enter name of material: '
      READ 5,  MAT
      PRINT *,' Enter density of material (g/cm3): '
      READ *, RHO
      NPHAS=2
      IF(RHO.LT.RHOCUT) NPHAS=1
      PRINT *,' Should the composition data be stored in a file?'
      PRINT *,'     (1 = yes; 2 = no): '
      READ *, ISTOR
      IF(ISTOR.EQ.2) GO TO 8
      PRINT *,' Enter name of this data file: '
      READ 5, OUTFIL
    8 PRINT *,' Options for type of material:'
      PRINT *,'     1) Element'
      PRINT *,'     2) Compound'
      PRINT *,'     3) Mixture of elements and/or compounds'
      PRINT *,' Choose 1, 2 or 3: '
      READ *, KMAT
      GO TO (10,12,20), KMAT
   10 PRINT *,' Enter chemical symbol for element: '
      GO TO 15
   12 PRINT *,' Enter chemical formula for compound: '
   15 READ 5,FORMLA
      CALL FORMEL(FORMLA,KMAT,NPHAS,MMAX,JZ,WT,ZAV,POT)
      GO TO 280
   20 PRINT *,' How many components in mixture? Enter number: '
      READ *,NCOMP
      DO 90 N=1,NCOMP
      PRINT 30, N
   30 FORMAT(' Choice for component',I3,': ')
      PRINT *,'     1) Use input from composition file UCOMP'
      PRINT *,'     2) Enter chemical formula'
      PRINT *,' Choose 1 or 2: '
      READ *,JINP
      JZIP(N)=0
      GO TO (40,50) JINP
   40 PRINT 45, N
   45 FORMAT(' Enter ID number for component',I3,': ')
      READ *, JZIP(N)
      CALL INDEX(JZIP(N),IDNO)
      FRM(N)=IDNO
      GO TO 70
   50 PRINT 60, N
   60 FORMAT(' Enter chemical symbol or formula for component',
     1 I3,': ')
      READ 5, FRM(N)
   70 PRINT 80, N
   80 FORMAT(' Enter fraction by weight for component',I3,': ')
      READ *, FRAC(N)
   90 CONTINUE
      PRINT 1
      SUMF=0.0
      DO 100 N=1,NCOMP
  100 SUMF=SUMF+FRAC(N)
      PRINT 110
  110 FORMAT('   Component    Fraction')
      PRINT 120
  120 FORMAT('                by Weight')
      DO 140 N=1,NCONP
      PRINT 130,N,FRAC(N),FRM(N)
  130 FORMAT(I12,F12.6,3X,A)
  140 CONTINUE
      PRINT 150, SUMF
  150 FORMAT(6X,'Sum = ',F12.6)
      PRINT 1
      PRINT *,' Options for accepting or rejecting composition data:'
      PRINT *,'     1. Accept, but let program normalize fractions'
      PRINT *,'        by weight so that their sum is unity'
      PRINT *,'     2. Reject, and enter different set of fractions'
      PRINT *,' Choose 1 or 2: '
      READ *, MSUMGO
      GO TO (160,20), MSUMGO
  160 DO 170 N=1,NCONP
  170 FRAC(N)=FRAC(N)/SUMF
      DO 180 L=1,100
  180 LH(L)=0
      DO 250 N=1,NCOMP
      IF(JZIP(N))190,190,200
  190 CALL FORMEL (FRM(N),KMAT,NPHAS,MAX,JZ1,WT1,ZAV1(N),POT1(N))
      GO TO 220
  200 JPIC=JZIP(N)
      IF(JPIC-278)210,210,201
  201 IF(JPIC-906)203,202,203
  202 JPIC=279
      GO TO 210
  203 PRINT 204, JPIC
  204 FORMAT(I6,' is not an allowed ID number.')
      STOP 4
  210 READ (4,REC=JPIC) MAT1,MAX,ZAV1,POT1,RHO1,JZ1,WT1
  220 DO 250 M=1,MAX
      IN=JZ1(M)
      IF(LH(IN))230,230,240
  230 LH(IN)=1
      WATE(IN)=FRAC(N)*WT1(M)
      GO TO 250
  240 WATE(IN)=WATE(IN)+FRAC(N)*WT1(M)
  250 CONTINUE
      LL=0
      DO 260 L=1,100
      IF(LH(L))260,260,255
  255 LL=LL+1
      JZ(LL)=L
      WT(LL)=WATE(L)
  260 CONTINUE
      MMAX=LL
      ZAV=0.0
      POTL=0.0
      DO 270 N=1,NCOMP
      ZAV=ZAV+FRAC(N)*ZAV1(N)
  270 POTL=POTL+FRAC(N)*ZAV1(N)*LOG(POT1(N))
      POT=EXP(POTL/ZAV)
  280 PRINT 290, POT
  290 FORMAT('  I-value computed by program is = ',F6.1,' eV.')
      PRINT *, ' Is this value acceptable (1=yes,2=no): '
      READ *, IPOT
      IF(IPOT.EQ.1) GO TO 295
      PRINT *,' Enter desired I-value (eV): '
      READ *, POT
  295 GO TO (300,340), ISTOR
  300 OPEN (UNIT=8,FILE=OUTFIL)
      WRITE (8,310) MAT
  310 FORMAT(1X,A)
      WRITE (8,320) MMAX,ZAV,POT,RHO
  320 FORMAT(I6,0P2F12.6,1PE12.5)
      WRITE (8,330) (JZ(M),WT(M),M=1,MMAX)
  330 FORMAT(6(I3,F9.6))
      CLOSE (8)
  340 RETURN
      END

      SUBROUTINE FORMEL (W,KMAT,NPHAS,MMAX,JZ,WT,ZAV,POT)
C     23 Jul 89. Interprets chemical formula.
C                Derived from FORM in XCOM, 24 Mar 87
C
C                W: chemical formula
C                KMAT: Phase index
C                MMAX: number of atomic constituents
C                JZ(M),M=1,MMAX: atomic numbers of constituents
C                WT(M),M-1,MMAX: fractions by weight
C                ZAV:  <Z/A>
C                POT: mean excitation energy of compound (eV)
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION MASH1(26),MASH2(418),IC(72),K(72),NZ(100),MS(100),
     1 ATWTD(100),POTGAS(9),POTCON(9),POTH(100),JZ(100),WT(100)
      CHARACTER W*72
      DATA MASH1/0,5,6,0,0,9,0,1,53,0,19,0,0,7,8,15,0,0,16,
     1 0,92,23,74,0,39,0/
      DATA (MASH2(I),I=1,111)/70,36*0,54,3*0,73,8*0,65,8*0,43,51,88,
     1 7*0,21,37,6*0,52,3*0,91,5*0,34,2*0,82,6*0,75,30,2*0,11,2*0,
     2 90,3*0,46,0,41/
      DATA (MASH2(I),I=112,205)/2*0,22,7*0,57,0,14,45,3*0,60,5*0,40,
     1 2*0,10,2*0,81,8*0,69,9*0,62,5*0,12,2*0,50,2*0,31,0,28,4*0,
     2 86,10*0,61,3*0,3,3*0,2,64,5*0,38/
      DATA (MASH2(I),I=206,288)/0,72,84,3*0,20,3*0,80,0,26,3*0,56,6*0,
     1 25,5*0,59,0,93,42,48,2*0,5 44,5*0,58,0,89,2*0,78,76,2*0,98,
     2 4,3*0,94,6*0,49,15*0,36,47,0,67/
      DATA (MASH2(I),I=289,418)/0,100,3*0,83,7*0,71,2*0,77,5*0,17,97,
     1 7*0,96,10*0,13,3*0,87,2*0,27,0,95,4*0,68,8*0,99,10*0,24,
     2 6*0,63,0,55,35,9*0,18,6*0,29,0,33,8*0,85,8*0,79,5*0,66/
      DATA (ATWTD(K),K=1,60)/
     1    1.00794D0,       4.002602D0,      6.941D0,         9.012182D0,
     2   10.811D0,        12.011D0,        14.00674D0,      15.9994D0,
     3   18.9984032D0,    20.1797D0,       22.989768D0,     24.3050D0,
     4   26.981539D0,     28.0855D0,       30.973762D0,     32.066D0,
     5   35.4527D0,       39.948D0,        39.0983D0,       40.078D0,
     6   44.955910D0,     47.88D0,         50.9415D0,       51.9961D0,
     7   54.93805D0,      55.847D0,        58.93320D0,      58.69D0,
     8   63.546D0,        65.39D0,         69.723D0,        72.61D0,
     9   74.92159D0,      78.96D0,         79.904D0,        83.80D0,
     1   85.4678D0,       87.62D0,         88.90585D0,      91.224D0,
     2   92.90638D0,      95.94D0,         97.9072D0,       101.07D0,
     3  102.9055D0,      106.42D0,        107.8682D0,      112.411D0,
     4  114.82D0,        118.710D0,       121.75D0,        127.60D0,
     5  126.90447D0,     131.29D0,        132.90543D0,     137.327D0,
     6  138.9055D0,      140.115D0,       140.90765D0,     144.24D0/
      DATA (ATWTD(K),K=61,100)/
     1  144.9127D0,      150.36D0,        151.965D0,       157.25D0,
     2  158.92534D0,     162.50D0,        164.93032D0,     167.26D0,
     3  168.93421D0,     173.04D0,        174.967D0,       178.49D0,
     4  180.9479D0,      183.85D0,        186.207D0,       190.2D0,
     5  192.22D0,        195.08D0,        196.96654D0,     200.59D0,
     6  204.3833D0,      207.2D0,         208.98037D0,     208.9824D0,
     7  209.9871D0,      222.0176D0,      223.0197D0,      226.0254D0,
```

```
     8  227.0278D0,      232.0381D0,      231.03588D0,     238.0289D0,
     9  237.0482D0,      239.0522D0,      243.0614D0,      247.0703D0,
     1  247.0703D0,      251.0796D0,      252.083D0,       257.0951D0/
      DATA POTH/19.2,41.8,40.0,63.7,76.0,78.0,82.0,95.0,
     1  115.,137.,149.,156.,166.,173.,173.,180.,159.29,
     2  188.,190.,191.,216.,233.,245.,257.,272.,286.,
     3  297.,311.,322.,330.,334.,350.,347.,348.,357.,
     4  352.,363.,366.,379.,393.,417.,424.,428.,441.,
     5  449.,470.,470.,469.,488.,488.,487.,485.,491.,
     6  482.,488.,491.,501.,523.,535.,546.,560.,574.,
     7  580.,591.,614.,628.,650.,658.,674.,684.,694.,
     8  705.,718.,727.,736.,746.,757.,790.,790.,800.,
     9  810.,823.,823.,830.,825.,794.,827.,826.,841.,
     1  847.,878.,890.,902.,921.,934.,939.,952.,966.,
     2  980.,994./
      DATA POTGAS/19.2,41.8,34.0,38.6,49.0,70.0,82.0,
     3  97.0,115.0/
      DATA POTCON/19.2,41.8,45.2,72.0,85.9,81.0,82.0,
     4  106.0,112.0/
      DO 116 L=1,72
      IC(L)=ICHAR(W(L:L))
      IF(IC(L)-32)101,102,103
  101 K(L)=1
      GO TO 116
  102 K(L)=2
      GO TO 116
  103 IF(IC(L)-48)104,105,105
  104 K(L)=1
      GO TO 116
  105 IF(IC(L)-58)106,107,107
  106 K(L)=3
      GO TO 116
  107 IF(IC(L)-65)108,109,109
  108 K(L)=1
      GO TO 116
  109 IF(IC(L)-91)110,111,111
  110 K(L)=4
      GO TO 116
  111 IF(IC(L)-97)112,113,113
  112 K(L)=1
      GO TO 116
  113 IF(IC(L)-123)114,115,115
  114 K(L)=5
      GO TO 116
  115 K(L)=1
  116 CONTINUE
      L=1
      M=0
  117 IF(K(L)-2)118,118,119
  118 L=L+1
      GO TO 117
  119 LMIN=L
  120 KG=K(L)
      IF(L-LMIN)130,130,140
  130 GO TO (150,150,150,160,150), KG
  140 GO TO (150,470,150,160,150), KG
  150 STOP 5
  160 KG1=K(L+1)
      GO TO (170,180,180,180,240), KG1
  170 STOP 6
  180 ICC=IC(L)-64
      JT=MASH1(ICC)
      IF(JT)190,190,200
  190 STOP 7
  200 M=M+1
      JZ(M)=JT
      GO TO (170,210,230,220,240), KG1
  210 NZ(M)=1
      GO TO 470
  220 NZ(M)=1
      L=L+1
      GO TO 120
  230 IN=L+1
      GO TO 390
  240 ICC=9*IC(L+1)-10*IC(L)+9
      IF(ICC-1)310,250,250
  250 IF(ICC-418)260,260,310
  260 IF(ICC-208)300,270,300
  270 M=M+1
      IF(IC(L)-71)290,280,290
  280 JZ(M)=32
      GO TO 330
  290 JZ(M)=84
      GO TO 330
  300 JT=MASH2(ICC)
      IF(JT)310,310,320
  310 STOP 8
  320 M=M+1
      JZ(M)=JT
  330 KG2=K(L+2)
      GO TO (340,350,380,360,370), KG2
  340 STOP 9
  350 NZ(M)=1
      GO TO 470
  360 NZ(M)=1
      L=L+2
      GO TO 120
  370 STOP 10
  380 IN=L+2
  390 INN=IN
      IS=0
      NZ(M)=0
  400 IF(K(INN)-3)420,410,420
  410 IS=IS+1
      MS(IS)=IC(INN)-48
      INN=INN+1
      GO TO 400
  420 ISM=IS
      KFAC=1
  430 NZ(M)=NZ(M)+KFAC*MS(IS)
      KFAC=10*KFAC
      IS=IS-1
      IF(IS)440,440,430
  440 IF(NZ(M))450,450,460
  450 STOP 12
  460 L=IN+ISM
      GO TO 120
  470 MMAX=M
      ASUM=0.0
      DO 480 M=1,MMAX
      JM=JZ(M)
  480 ASUM=ASUM+ATWTD(JM)*DBLE(NZ(M))
      DO 490 M=1,MMAX
      JM=JZ(M)
  490 WT(M)=ATWTD(JM)*DBLE(NZ(M))/ASUM
      ZAV=0.0
      POTL=0.0
      DO 540 M=1,MMAX
      JM=JZ(M)
      ZA=DBLE(JZ(M))/ATWTD(JM)
      ZAV=ZAV+WT(M)*ZA
      IF(KHAT-1)492,492,495
  492 POTH=POTH(JM)
      GO TO 540
  495 IF(JM-10)500,530,530
  500 GO TO (510,520), NPHAS
  510 POTH=POTGAS(JM)
      GO TO 540
  520 POTH=POTCON(JM)
      GO TO 540
  530 POTH=1.13*POTH(JM)
  540 POTL=POTL+WT(M)*ZA*LOG(POTH)
      POT=EXP(POTL/ZAV)
      RETURN
      END

      SUBROUTINE INDEX (L,TAG)
      CHARACTER TAG*3,IND(0:9)*1
      DATA IND/'0','1','2','3','4','5','6','7','8','9'/
      I1=L/100
      M=L-100*I1
      I2=M/10
      I3=M-10*I2
      TAG=IND(I1)//IND(I2)//IND(I3)
      RETURN
      END

      SUBROUTINE SCOF(X,F,NMAX,A,B,C,D)
C     22 Feb 83
C  IF S LIES BETWEEN X(M) AND X(M+1), THEN
C  F(S)=((D(M)*S+C(M))*S+B(M))*S+A(M)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(1000),F(1000),A(1000),B(1000),C(1000),D(1000)
      M1=2
      M2=NMAX-1
      S=0.0
      DO 10 M=1,M2
      D(M)=X(M+1)-X(M)
      R=(F(M+1)-F(M))/D(M)
      C(M)=R-S
   10 S=R
      S=0.0
      R=0.0
      C(1)=0.0
      C(NMAX)=0.0
      DO 20 M=M1,M2
      C(M)=C(M)+R*C(M-1)
      B(M)=(X(M-1)-X(M+1))*2.0-R*S
      S=D(M)
   20 R=S/B(M)
      MR=M2
      DO 30 M=M1,M2
      C(MR)=(D(MR)*C(MR+1)-C(MR))/B(MR)
   30 MR=MR-1
      DO 40 M=1,M2
      S=D(M)
      R=C(M+1)-C(M)
      D(M)=R/S
      C(M)=C(M)*3.0
      B(M)=(F(M+1)-F(M))/S-(C(M)+R)*S
   40 A(M)=F(M)
      RETURN
```

```
      END

      SUBROUTINE BSPOL(S,X,A,B,C,D,N,G)
C     22 FEB 83
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(1000),A(1000),B(1000),C(1000),D(1000)
      IF (X(1).GT.X(N)) GO TO 10
      IDIR=0
      MLB=0
      MUB=N
      GO TO 20
   10 IDIR=1
      MLB=N
      MUB=0
   20 IF (S.GE.X(MUB+IDIR)) GO TO 60
      IF (S.LE.X(MLB+1-IDIR)) GO TO 70
      ML=MLB
      MU=MUB
      GO TO 40
   30 IF (IABS(MU-ML).LE.1) GO TO 80
   40 MAV=(ML+MU)/2
      IF (S.LT.X(MAV)) GO TO 50
      ML=MAV
      GO TO 30
   50 MU=MAV
      GO TO 30
   60 MU=MUB+2*IDIR-1
      GO TO 90
   70 MU=MLB-2*IDIR+1
      GO TO 90
   80 MU=MU+IDIR-1
   90 Q=S-X(MU)
      G=((D(MU)*Q+C(MU))*Q+B(MU))*Q+A(MU)
      RETURN
      END

      SUBROUTINE GRAL(DELTA,G,N,RESULT)
C     SUBROUTINE GRAL(DELTA,G,N,RESULT); 5 MAY 86; FORMERLY INT
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION G(10001)
      NL1=N-1
      NL2=N-2
      IF (FLOAT (N) -2.0*FLOAT (N/2)) 100,100,10
C     IF N IS ODD, GO TO 10 - IF N IS EVEN, GO TO 100
   10  IF (N-1) 15,15,20
   15 SIGMA=0.0
      GO TO 70
   20 IF(N-3) 30,30,40
   30 SIGMA=G(1)+4.0*G(2)+G(3)
      GO TO 70
   40 SUM4=0.0
      DO 50 K=2,NL1,2
   50 SUM4=SUM4+G(K)
      SUM2=0.0
      DO 60 K=3,NL2,2
   60 SUM2=SUM2+G(K)
      SIGMA=G(1)+4.0*SUM4+2.0*SUM2+G(N)
   70 RESULT=DELTA*SIGMA
      RETURN
  100 IF(N-2)110,110,120
  110 SIGMA=1.5*(G(1)+G(2))
      GO TO 70
  120 IF(N-4)130,130,140
  130 SIGMA=1.125*(G(1)+3.0*G(2)+3.0*G(3)+G(4))
      GO TO 70
  140 IF(N-6)150,150,160
  150 SIGMA=G(1)+3.875*G(2)+2.625*G(3)+2.625*G(4)+3.875*G(5)+G(6)
      GO TO 70
  160 IF (N-8)170,170,180
  170 SIGMA=G(1)+3.875*G(2)+2.625*G(3)+2.625*G(4)+3.875*G(5)+2.0*G(6)
     1+4.0*G(7)+G(8)
      GO TO 70
  180 SIG6=G(1)+3.875*G(2)+2.625*G(3)+2.625*G(4)+3.875*G(5)+G(6)
      SUM4=0.0
      DO 190 K=7,NL1,2
  190 SUM4=SUM4+G(K)
      SUM2=0.0
      DO 200 K=8,NL2,2
  200 SUM2=SUM2+G(K)
      SIGMA=SIG6+G(6)+4.0*SUM4+2.0*SUM2+G(N)
      GO TO 70
      END
```

```
      PROGRAM PSTAR
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
C     PSTAR produces table of proton stopping powers, ranges
C     detour factors, and average penetration depths, at a chosen set of
C     energies. Energies can be entered from keyboard, or from prepared
C     energy-list file. Such a file must contain, in the first record,
C     the number of energies, and in next record(s) the energies
C     (in MeV) separated by blanks.
C
C     PSTAR calls subroutine PPOL, which in turn calls
C     subroutines PREAD, SCOF and BSPOL.
C
C     PSTAR uses input from the direct-access binary file UPROT.
C
      DIMENSION T(1000),STOPEL(1000),STOPNUC(1000),STOPTOT(1000),
     1 RANGE(1000),DETOUR(1000),AVPEN(1000),IDNO(74)
      CHARACTER TAG*72,NAME(74)*72,ENGIN*30,OUTPUT*30
      DATA IDNO/ 1,  2,  4,  6,906,  7,  8, 10, 13, 14, 18, 22, 26,
     1          29, 32, 36, 42, 47, 50, 54, 64, 74, 78, 79, 82, 92,
     2         99,101,103,104,106,111,119,120,126,130,134,138,139,
     3        141,155,160,169,179,185,189,191,197,200,201,202,203,
     4        204,209,213,215,216,219,221,222,223,225,226,227,232,
     5        238,245,252,255,263,264,266,276,277/
    1 FORMAT(1H )
    5 FORMAT(A)
      OPEN (UNIT=7,FILE='MATS')
      DO 10 J=1,74
   10 READ (7,5) NAME(J)
      CLOSE (7)
      PRINT *,' Enter ID number of material: '
      READ *, ID
      DO 20 I=1,74
      IF(IDNO(I).EQ.ID) GO TO 35
   20 CONTINUE
      PRINT 30, ID
   30 FORMAT(I6,' is not one of the ID numbers in database PSTAR.')
      STOP
   35 TAG=NAME(I)
      PRINT *,' Choice for energy-list input: '
      PRINT *,'    1) Use default file ENG.PRO'
      PRINT *,'    2) Use prepared file'
      PRINT *,'    3) Entry from keyboard'
      PRINT *,' Choose 1, 2, or 3: '
      READ *, INENG
      GO TO (40,50,70), INENG
   40 ENGIN='ENG.PRO'
      OPEN (UNIT=7,FILE=ENGIN)
      READ (7,*) LMAX
      READ (7,*) (T(L),L=1,LMAX)
      CLOSE (7)
      GO TO 75
   50 PRINT *,' Enter name of energy-list file: '
      READ 5, ENGIN
      OPEN (UNIT=7,FILE=ENGIN)
      READ (7,*) LMAX
      READ (7,*) (T(L),L=1,LMAX)
      CLOSE (7)
   55 TMIN=1.0E12
      TMAX=0.0
      DO 60 L=1,LMAX
      IF(T(L).LT.TMIN) TMIN=T(L)
      IF(T(L).GT.TMAX) TMAX=T(L)
   60 CONTINUE
      IF(TMIN-0.001)62,64,64
   62 PRINT 63
   63 FORMAT(' At least one of the energies is below 0.001 MeV, out of r
     1ange.')
      STOP
   64 IF(TMAX-10000.0)75,75,65
   65 PRINT 66
   66 FORMAT(' At least one of the energies is above 10000.0 MeV, out of
     1 range.')
      STOP
   70 PRINT *,' How many energies?  '
      READ *, LMAX
      PRINT *,' Enter energies (in MeV): '
      READ *, (T(L),L=1,LMAX)
      GO TO 55
   75 PRINT *,' Enter name of output file: '
      READ 5, OUTPUT
      OPEN (UNIT=8,FILE=OUTPUT)
      CALL PPOL(ID,LMAX,T,STOPEL,STOPNUC,STOPTOT,RANGE,DETOUR,AVPEN)
      WRITE (8,80)
   80 FORMAT(' PROTON STOPPING POWER AND RANGE')
      WRITE (8,1)
      WRITE (8,90)
   90 FORMAT('    ID number')
      WRITE (8,100) ID,TAG
  100 FORMAT(I12,3X,A)
      WRITE (8,1)
      WRITE (8,110)
  110 FORMAT('         T = Proton energy, MeV')
      WRITE (8,120)
  120 FORMAT('  STOP(e) = electronic stopping power, MeV cm2/g')
      WRITE (8,130)
  130 FORMAT('  STOP(n) = nuclear stopping power, MeV cm2/g')
      WRITE (8,140)
  140 FORMAT('  STOP(t) = total stopping power, MeV cm2/g')
      WRITE (8,150)
  150 FORMAT(' RANGE(c) = csda range, g/cm2')
      WRITE (8,160)
  160 FORMAT(' RANGE(p) = projected range, g/cm2')
      WRITE (8,170)
  170 FORMAT('    DETOUR = detour factor')
      WRITE (8,1)
      WRITE (8,180)
  180 FORMAT(10X,'T',4X,'STOP(e)',4X,'STOP(n)',4X,'STOP(t)',
     1 3X,'RANGE(c)',3X,'RANGE(p)',2X,'DETOUR')
      WRITE (8,1)
      DO 200 L=1,LMAX
      WRITE (8,190) T(L),STOPEL(L),STOPNUC(L),STOPTOT(L),RANGE(L),
     1 AVPEN(L),DETOUR(L)
  190 FORMAT(0PF11.4,1P5E11.3,0PF8.4)
  200 CONTINUE
      STOP
      END

      SUBROUTINE PREAD (ID,STE,STN,RG,DET)
C     22 Jun 91. Reads binary direct-access file UPROT for protons.
C
C       Input argument:
C           ID:  Identification number of material.
C
C     Output arguments:
C
C          STE:  Array of NMAX electronic stopping powers, in MeV cm2/g
C          STN:  Array of NMAX nuclear stopping powers, in MeV cm2/g
C           RG:  Array of NMAX csda ranges, in g/cm2
C          DET:  Array of NMAX detour factors
C
      DIMENSION STE(133),STN(133),RG(133),DET(133),IND(74)
      DATA IND/  1,  2,  4,  6,  7,  8, 10, 13, 14, 18, 22, 26, 29, 32,
     1          36, 42, 47, 50, 54, 64, 74, 78, 79, 82, 92, 99,101,103,
     2         104,106,111,119,120,126,130,134,138,139,141,155,160,169,
     3         179,185,189,191,197,200,201,202,203,204,209,213,215,216,
     4         219,221,222,223,225,226,227,232,238,245,252,255,263,264,
     3         266,276,277,906/
      DO 10 J=1,74
      IF(ID.EQ.IND(J)) GO TO 30
   10 CONTINUE
      PRINT 20, ID
   20 FORMAT(I6,' is not a permitted ID number.')
      STOP
   30 JD=J
      OPEN (UNIT=7,FILE='UPROT',FORM='UNFORMATTED',
     1 ACCESS='DIRECT',RECL=2128)
      READ (7,REC=JD) STE,STN,RG,DET
      CLOSE (7)
      RETURN
      END

      SUBROUTINE PPOL(ID,LMAX,T,STOPEL,STOPNUC,STOPTOT,RANGE,DETOUR,
     1 AVPEN)
C     22 June 1991
C
C     Subroutine PPOL calculates, by interpolation, proton
C     stopping powers, rnges, detour factors and average penetration
C     depths, at specified energies (between 1 keV and 10000 MeV).
C
C     Input arguments:
C             ID:  Identification number of material
C           LMAX:  Number of energies
C              T:  Array of LMAX energies, in MeV
C
C     Output arguments:
C          STOPEL:  Array of LMAX electronic stopping powers, in MeV cm2/g
C          STOPNUC:  Array of LMAX nuclear stopping powers, in MeV cm2/g
C          STOPTOT:  Array of LMAX total stopping powers, in MeV cm2/g
C            RANGE:  Array of LMAX csda ranges, in g/cm2
C           DETOUR:  Array of LMAX detour factors
C            AVPEN:  Array of LMAX average penetration depths, in g/cm2
C
      DIMENSION E(133),EL(133),STE(133),STEL(133),STN(133),STNL(133),
     1 RG(133),RGL(133),DET(133),DETL(133),AF(133),BF(133),CF(133),
     2 DF(133),T(1000),TL(1000),STOPEL(1000),STOPNUC(1000),
     3 STOPTOT(1000),RANGE(1000),DETOUR(1000),AVPEN(1000)
      DATA E/
     1 0.0010,0.0015,0.0020,0.0025,0.0030,0.0040,0.0050,0.0060,0.0070,
     2 0.0080,0.0090,0.0100,0.0125,0.0150,0.0175,0.0200,0.0225,0.0250,
     3 0.0275,0.0300,0.0350,0.0400,0.0450,0.0500,0.0550,0.0600,0.0650,
     4 0.0700,0.0750,0.0800,0.0850,0.0900,0.0950,0.1000,0.1250,0.1500,
     5 0.1750,0.2000,0.2250,0.2500,0.2750,0.3000,0.3500,0.4000,0.4500,
     6 0.5000,0.5500,0.6000,0.6500,0.7000,0.7500,0.8000,0.8500,0.9000,
     7 0.9500,1.0000,1.2500,1.5000,1.7500,2.0000,2.2500,2.5000,2.7500,
     8 3.0000,3.5000,4.0000,4.5000,5.0000,5.5000,6.0000,6.5000,7.0000,
     9 7.5000,8.0000,8.5000,9.0000,9.5000,10.0000,12.5000,15.0000,
```

```
     1 17.5000,20.0000,22.5000,25.0000,27.5000,30.0000,35.0000,40.0000,
     2 45.0000,50.0000,55.0000,60.0000,65.0000,70.0000,75.0000,80.0000,
     2 85.0000,90.0000,95.0000,100.0,125.0,150.0,175.0,200.0,225.0,
     3 250.0,275.0,300.0,350.0,400.0,450.0,500.0,550.0,600.0,650.0,
     5 700.0,750.0,800.0,850.0,900.0,950.0,1000.0,1500.0,2000.0,2500.0,
     6 3000.0,4000.0,5000.0,6000.0,7000.0,8000.0,9000.0,10000.0/
      DATA NMAX/133/
      CALL PREAD(ID,STE,STN,RG,DET)
      DO 10 L=1,LMAX
      IF(T(L).GT.10000.0) GO TO 70
      IF(T(L).LT.0.001) GO TO 70
   10 TL(L)=LOG(T(L))
      DO 20 N=1,NMAX
      EL(N)=LOG(E(N))
      STEL(N)=LOG(STE(N))
      STNL(N)=LOG(STN(N))
      RGL(N)=LOG(RG(N))
   20 DETL(N)=LOG(DET(N))
      CALL SCOF(EL,STEL,NMAX,AF,BF,CF,DF)
      DO 30 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
   30 STOPEL(L)=EXP(RES)
      CALL SCOF(EL,STNL,NMAX,AF,BF,CF,DF)
      DO 40 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
      STOPNUC(L)=EXP(RES)
   40 STOPTOT(L)=STOPEL(L)+STOPNUC(L)
      CALL SCOF(EL,RGL,NMAX,AF,BF,CF,DF)
      DO 50 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
   50 RANGE(L)=EXP(RES)
      CALL SCOF(EL,DETL,NMAX,AF,BF,CF,DF)
      DO 60 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
      DETOUR(L)=EXP(RES)
   60 AVPEN(L)=DETOUR(L)*RANGE(L)
      RETURN
   70 PRINT 80,T(L)
   80 FORMAT(' Input energy ',1PE12.5,' out of range.')
      RETURN
      END

      SUBROUTINE SCOF(X,F,NMAX,A,B,C,D)
C     SUBRROUTINE SCOF(X,F,NMAX,A,B,C,D), 22 FEB 83
C  IF S LIES BETWEEN X(M) AND X(M+1), THEN
C  F(S)=((D(M)*S+C(M))*S+B(M))*S+A(M)
      DIMENSION X(1000),F(1000),A(1000),B(1000),C(1000),D(1000)
      M1=2
      M2=NMAX-1
      S=0.0
      DO 10 M=1,M2
      D(M)=X(M+1)-X(M)
      R=(F(M+1)-F(M))/D(M)
      C(M)=R-S
   10 S=R
      S=0.0
      R=0.0
      C(1)=0.0
      C(NMAX)=0.0
      DO 20 M=M1,M2
      C(M)=C(M)+R*C(M-1)
      B(M)=(X(M-1)-X(M+1))*2.0-R*S
      S=D(M)
   20 R=S/B(M)
      MR=M2
      DO 30 M=M1,M2
      C(MR)=(D(MR)*C(MR+1)-C(MR))/B(MR)
   30 MR=MR-1
      DO 40 M=1,M2
      S=D(M)
      R=C(M+1)-C(M)
      D(M)=R/S
      C(M)=C(M)*3.0
      B(M)=(F(M+1)-F(M))/S-(C(M)+R)*S
   40 A(M)=F(M)
      RETURN
      END

      SUBROUTINE BSPOL(S,X,A,B,C,D,N,G)
C     SUBROUTINE BSPOL(S,X,A,B,C,D,N,G), 22 FEB 83
      DIMENSION X(1000),A(1000),B(1000),C(1000),D(1000)
      IF (X(1).GT.X(N)) GO TO 10
      IDIR=0
      MLB=0
      MUB=N
      GO TO 20
   10 IDIR=1
      MLB=N
      MUB=0
   20 IF (S.GE.X(MUB+IDIR)) GO TO 60
      IF (S.LE.X(MLB+1-IDIR)) GO TO 70
      ML=MLB
      MU=MUB
      GO TO 40
   30 IF (IABS(MU-ML).LE.1) GO TO 80
   40 MAV=(ML+MU)/2
      IF (S.LT.X(MAV)) GO TO 50
      ML=MAV
      GO TO 30
   50 MU=MAV
      GO TO 30
   60 MU=MUB+2*IDIR-1
      GO TO 90
   70 MU=MLB-2*IDIR+1
      GO TO 90
   80 MU=MU+IDIR-1
   90 Q=S-X(MU)
      G=((D(MU)*Q+C(MU))*Q+B(MU))*Q+A(MU)
      RETURN
      END
```

```
      PROGRAM ASTAR
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
C     ASTAR produces table of alpha-particle stopping powers, ranges,
C     detour factors, and average penetration depths, at a chosen set of
C     energies. Energies can be entered from keyboard, or from a prepared
C     energy-list file. Such a file must contain, in the first record,
C     the number of energies, and in the next record(s) the energies
C     (in MeV) separated by blanks.
C
C     ASTAR calls subroutine APOL, which in turn calls
C     subroutines AREAD, SCOF and BSPOL.
C
C     ASTAR uses input from the direct-access binary file UALPH.
C
      DIMENSION T(1000),STOPEL(1000),STOPNUC(1000),STOPTOT(1000),
     1 RANGE(1000),DETOUR(1000),AVPEN(1000),IDNO(74)
      CHARACTER TAG*72,NAME(74)*72,ENGIN*30,OUTPUT*30
      DATA IDNO/ 1,  2,  4,  6,906,  7,  8, 10, 13, 14, 18, 22, 26,
     1          29, 32, 36, 42, 47, 50, 54, 64, 74, 78, 79, 82, 92,
     2          99,101,103,104,106,111,119,120,126,130,134,138,139,
     3         141,155,160,169,179,185,189,191,197,200,201,202,203,
     4         204,209,213,215,216,219,221,222,223,225,226,227,232,
     5         238,245,252,255,263,264,266,276,277/
    1 FORMAT(1H )
    5 FORMAT(A)
      OPEN (UNIT=7,FILE='MATS')
      DO 10 J=1,74
   10 READ (7,5) NAME(J)
      CLOSE (7)
      PRINT *,' Enter ID number of material: '
      READ *, ID
      DO 20 I=1,74
      IF(IDNO(I).EQ.ID) GO TO 35
   20 CONTINUE
      PRINT 30, ID
   30 FORMAT(I6,' is not one of the ID numbers in database ASTAR.')
      STOP
   35 TAG=NAME(I)
      PRINT *,' Choice for energy-list input: '
      PRINT *,'    1) Use default file ENG.ALF'
      PRINT *,'    2) Use prepared file'
      PRINT *,'    3) Entry from keyboard'
      PRINT *,' Choose 1, 2, or 3: '
      READ *, INENG
      GO TO (40,50,70), INENG
   40 ENGIN='ENG.ALF'
      OPEN (UNIT=7,FILE=ENGIN)
      READ (7,*) LMAX
      READ (7,*) (T(L),L=1,LMAX)
      CLOSE (7)
      GO TO 75
   50 PRINT *,' Enter name of energy-list file: '
      READ 5, ENGIN
      OPEN (UNIT=7,FILE=ENGIN)
      READ (7,*) LMAX
      READ (7,*) (T(L),L=1,LMAX)
      CLOSE (7)
   55 TMIN=1.0E12
      TMAX=0.0
      DO 60 L=1,LMAX
      IF(T(L).LT.TMIN) TMIN=T(L)
      IF(T(L).GT.TMAX) TMAX=T(L)
   60 CONTINUE
      IF(TMIN-0.001)62,64,64
   62 PRINT 63
   63 FORMAT(' At least one of the specified energies is below 0.001 MeV
     1, out or range.')
      STOP
   64 IF(TMAX-1000.0)75,75,65
   65 PRINT 66
   66 FORMAT(' At least one of the specified energies is above 0.001 MeV
     1, out or range.')
      STOP
   70 PRINT *,' How many energies?  '
      READ *, LMAX
      PRINT *,' Enter energies (in MeV): '
      READ *, (T(L),L=1,LMAX)
      GO TO 55
   75 PRINT *,' Enter name of output file: '
      READ 5, OUTPUT
      OPEN (UNIT=8,FILE=OUTPUT)
      CALL APOL(ID,LMAX,T,STOPEL,STOPNUC,STOPTOT,RANGE,DETOUR,AVPEN)
      WRITE (8,80)
   80 FORMAT(' ALPHA PARTICLE STOPPING POWER AND RANGE')
      WRITE (8,1)
      WRITE (8,90)
   90 FORMAT('   ID number')
      WRITE (8,100) ID,TAG
  100 FORMAT(I12,3X,A)
      WRITE (8,1)
      WRITE (8,110)
  110 FORMAT('        T = alpha particle (helium ion) energy, MeV')
      WRITE (8,120)
  120 FORMAT('  STOP(e) = electronic stopping power, MeV cm2/g')
      WRITE (8,130)
  130 FORMAT('  STOP(n) = nuclear stopping power, MeV cm2/g')
      WRITE (8,140)
  140 FORMAT('  STOP(t) = total stopping power, MeV cm2/g')
      WRITE (8,150)
  150 FORMAT(' RANGE(c) = csda range, g/cm2')
      WRITE (8,160)
  160 FORMAT(' RANGE(p) = projected range, g/cm2')
      WRITE (8,170)
  170 FORMAT('   DETOUR = detour factor')
      WRITE (8,1)
      WRITE (8,180)
  180 FORMAT(10X,'T',4X,'STOP(e)',4X,'STOP(n)',4X,'STOP(t)',
     1 3X,'RANGE(c)',3X,'RANGE(p)',2X,'DETOUR')
      WRITE (8,1)
      DO 200 L=1,LMAX
      WRITE (8,190) T(L),STOPEL(L),STOPNUC(L),STOPTOT(L),RANGE(L),
     1 AVPEN(L),DETOUR(L)
  190 FORMAT(0PF11.4,1P5E11.3,0PF8.4)
  200 CONTINUE
      STOP
      END

      SUBROUTINE AREAD (ID,STE,STN,RG,DET)
C     22 Jun 91. Reads binary direct-access file UALPH
C                for alpha particles.
C
C       Input argument:
C           ID:  Identification number of material.
C
C     Output arguments:
C
C          STE:  Array of NMAX electronic stopping powers, in MeV cm2/g
C          STN:  Array of NMAX nuclear stopping powers, in MeV cm2/g
C           RG:  Array of NMAX csda ranges, in g/cm2
C          DET:  Array of NMAX detour factors
C
      DIMENSION STE(122),STN(122),RG(122),DET(122),IND(74)
      DATA IND/  1,  2,  4,  6,  7,  8, 10, 13, 14, 18, 22, 26, 29, 32,
     1          36, 42, 47, 50, 54, 64, 74, 78, 79, 82, 92, 99,101,103,
     2         104,106,111,119,120,126,130,134,138,139,141,155,160,169,
     3         179,185,189,191,197,200,201,202,203,204,209,213,215,216,
     4         219,221,222,223,225,226,227,232,238,245,252,255,263,264,
     3         266,276,277,906/
      DO 10 J=1,74
      IF(ID.EQ.IND(J)) GO TO 30
   10 CONTINUE
      PRINT 20, ID
   20 FORMAT(I6,' is not a permitted ID number.')
      STOP
   30 JD=J
      OPEN (UNIT=7,FILE='UALPH',FORM='UNFORMATTED',
     1 ACCESS='DIRECT',RECL=1952)
      READ (7,REC=JD) STE,STN,RG,DET
      RETURN
      END

      SUBROUTINE APOL(ID,LMAX,T,STOPEL,STOPNUC,STOPTOT,RANGE,DETOUR,
     1 AVPEN)
C     22 June 1991.
C
C     Subroutine APOL calculates, by interpolation, alpha-particle
C     stopping powers, ranges, detour factors and average penetration
C     depths, at specified energies (between 1 keV and 1000 MeV).
C
C     Input arguments:
C             ID:  Identification number of material
C           LMAX:  Number of energies
C              T:  Array of LMAX energies, in MeV
C
C     Output arguments:
C          STOPEL:  Array of LMAX electronic stopping powers, in MeV cm2/g
C          STOPNUC:  Array of LMAX nuclear stopping powers, in MeV cm2/g
C          STOPTOT:  Array of LMAX total stopping powers, in MeV cm2/g
C            RANGE:  Array of LMAX csda ranges, in g/cm2
C           DETOUR:  Array of LMAX detour factors
C            AVPEN:  Array of LMAX average penetration depths, in g/cm2
C
      DIMENSION E(122),EL(122),STE(122),STEL(122),STN(122),STNL(122),
     1 RG(122),RGL(122),DET(122),DETL(122),AF(122),BF(122),CF(122),
     2 DF(122),T(1000),TL(1000),STOPEL(1000),STOPNUC(1000),
     3 STOPTOT(1000),RANGE(1000),DETOUR(1000),AVPEN(1000)
      DATA E/
     1 0.0010,0.0015,0.0020,0.0025,0.0030,0.0040,0.0050,0.0060,0.0070,
     2 0.0080,0.0090,0.0100,0.0125,0.0150,0.0175,0.0200,0.0225,0.0250,
     3 0.0275,0.0300,0.0350,0.0400,0.0450,0.0500,0.0550,0.0600,0.0650,
     4 0.0700,0.0750,0.0800,0.0850,0.0900,0.0950,0.1000,0.1250,0.1500,
     5 0.1750,0.2000,0.2250,0.2500,0.2750,0.3000,0.3500,0.4000,0.4500,
     6 0.5000,0.5500,0.6000,0.6500,0.7000,0.7500,0.8000,0.8500,0.9000,
     7 0.9500,1.0000,1.2500,1.5000,1.7500,2.0000,2.2500,2.5000,2.7500,
     8 3.0000,3.5000,4.0000,4.5000,5.0000,5.5000,6.0000,6.5000,7.0000,
     9 7.5000,8.0000,8.5000,9.0000,9.5000,10.0000,12.5000,15.0000,
```

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     1 17.5000,20.0000,22.5000,25.0000,27.5000,30.0000,35.0000,40.0000,
     2 45.0000,50.0000,55.0000,60.0000,65.0000,70.0000,75.0000,80.0000,
     2 85.0000,90.0000,95.0000,100.0,125.0,150.0,175.0,200.0,225.0,
     3 250.0,275.0,300.0,350.0,400.0,450.0,500.0,550.0,600.0,650.0,
     5 700.0,750.0,800.0,850.0,900.0,950.0,1000.0/
      DATA NMAX/122/
      CALL AREAD(ID,STE,STN,RG,DET)
      DO 10 L=1,LMAX
      IF(T(L).GT.1000.0) GO TO 70
      IF(T(L).LT.0.001) GO TO 70
   10 TL(L)=LOG(T(L))
      DO 20 N=1,NMAX
      EL(N)=LOG(E(N))
      STEL(N)=LOG(STE(N))
      STNL(N)=LOG(STN(N))
      RGL(N)=LOG(RG(N))
   20 DETL(N)=LOG(DET(N))
      CALL SCOF(EL,STEL,NMAX,AF,BF,CF,DF)
      DO 30 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
   30 STOPEL(L)=EXP(RES)
      CALL SCOF(EL,STNL,NMAX,AF,BF,CF,DF)
      DO 40 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
      STOPNUC(L)=EXP(RES)
   40 STOPTOT(L)=STOPEL(L)+STOPNUC(L)
      CALL SCOF(EL,RGL,NMAX,AF,BF,CF,DF)
      DO 50 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
   50 RANGE(L)=EXP(RES)
      CALL SCOF(EL,DETL,NMAX,AF,BF,CF,DF)
      DO 60 L=1,LMAX
      CALL BSPOL(TL(L),EL,AF,BF,CF,DF,NMAX,RES)
      DETOUR(L)=EXP(RES)
   60 AVPEN(L)=DETOUR(L)*RANGE(L)
      RETURN
   70 PRINT 80,T(L)
   80 FORMAT(' Input energy ',1PE12.5,' out of range.')
      RETURN
      END

      SUBROUTINE SCOF(X,F,NMAX,A,B,C,D)
C     SUBRROUTINE SCOF(X,F,NMAX,A,B,C,D), 22 FEB 83
C  IF S LIES BETWEEN X(M) AND X(M+1), THEN
C  F(S)=((D(M)*S+C(M))*S+B(M))*S+A(M)
      DIMENSION X(1000),F(1000),A(1000),B(1000),C(1000),D(1000)
      M1=2
      M2=NMAX-1
      S=0.0
      DO 10 M=1,M2
      D(M)=X(M+1)-X(M)
      R=(F(M+1)-F(M))/D(M)
      C(M)=R-S
   10 S=R
      S=0.0
      R=0.0
      C(1)=0.0
      C(NMAX)=0.0
      DO 20 M=M1,M2
      C(M)=C(M)+R*C(M-1)
      B(M)=(X(M-1)-X(M+1))*2.0-R*S
      S=D(M)
   20 R=S/B(M)
      MR=M2
      DO 30 M=M1,M2
      C(MR)=(D(MR)*C(MR+1)-C(MR))/B(MR)
   30 MR=MR-1
      DO 40 M=1,M2
      S=D(M)
      R=C(M+1)-C(M)
      D(M)=R/S
      C(M)=C(M)*3.0
      B(M)=(F(M+1)-F(M))/S-(C(M)+R)*S
   40 A(M)=F(M)
      RETURN
      END

      SUBROUTINE BSPOL(S,X,A,B,C,D,N,G)
C     SUBROUTINE BSPOL(S,X,A,B,C,D,N,G), 22 FEB 83
      DIMENSION X(1000),A(1000),B(1000),C(1000),D(1000)
      IF (X(1).GT.X(N)) GO TO 10
      IDIR=0
      MLB=0
      MUB=N
      GO TO 20
   10 IDIR=1
      MLB=N
      MUB=0
   20 IF (S.GE.X(MUB+IDIR)) GO TO 60
      IF (S.LE.X(MLB+1-IDIR)) GO TO 70
      ML=MLB
      MU=MUB
      GO TO 40
   30 IF (IABS(MU-ML).LE.1) GO TO 80
   40 MAV=(ML+MU)/2
      IF (S.LT.X(MAV)) GO TO 50
      ML=MAV
      GO TO 30
   50 MU=MAV
      GO TO 30
   60 MU=MUB+2*IDIR-1
      GO TO 90
   70 MU=MLB-2*IDIR+1
      GO TO 90
   80 MU=MU+IDIR-1
   90 Q=S-X(MU)
      G=((D(MU)*Q+C(MU))*Q+B(MU))*Q+A(MU)
      RETURN
      END
```

```
      PROGRAM COMPOS
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION MZ(14),WT(14)
      CHARACTER MAT*72,OUTPUT*30
    1 FORMAT(1H )
    5 FORMAT(A)
    6 FORMAT(1X,A)
      PRINT *,' Enter ID number: '
      READ *, ID
      PRINT *,' Enter name of output file (CON = monitor screen): '
      READ 5, OUTPUT
      OPEN (8,OUTPUT)
      IF(ID-278)50,50,10
   10 IF(ID-906)30,20,30
   20 ID=279
      GO TO 50
   30 PRINT 40, ID
   40 FORMAT(16,' is not an allowed ID number.')
      STOP
   50 OPEN (7,'UCOMP',FORM='UNFORMATTED',ACCESS='DIRECT',RECL=268)
      READ (7,REC=ID) MAT,MMAX,ZAG,POT,RHO,MZ,WT
      WRITE (8,55) ID
   55 FORMAT(' ID number ',I3)
      WRITE (8,1)
      WRITE (8,6) MAT
      WRITE (8,1)
      WRITE (8,60) RHO
   60 FORMAT('              Density (g/cm3) = ',F12.5)
      WRITE (8,1)
      WRITE (8,70) POT
   70 FORMAT(' Mean Excitation Energy (eV) = ',F8.1)
      WRITE (8,1)
      WRITE (8,80)
   80 FORMAT(' COMPOSITION:')
      WRITE (8,90)
   90 FORMAT('        Z = Atomic number')
      WRITE (8,100)
  100 FORMAT('       WT = fraction by weight')
      WRITE (8,1)
      WRITE (8,110)
  110 FORMAT(15X,'Z',8X,'WT')
      DO 130 M=1,MMAX
      WRITE (8,120) MZ(M),WT(M)
  120 FORMAT(10X,I6,F10.6)
  130 CONTINUE
      STOP
      END
      PROGRAM CONVERT
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION MZ(14),WT(14)
      CHARACTER MAT*72
      DATA KMAX/279/
    5 FORMAT(1X,A)
      OPEN (7,'FCOMP')
      OPEN (8,'UCOMP',FORM='UNFORMATTED',ACCESS='DIRECT',RECL=268)
      DO 20 K=1,KMAX
      READ (7,5) MAT
      READ (7,*) MMAX,ZAG,POT,RHO
      READ (7,10) (MZ(M),WT(M),M=1,MMAX)
   10 FORMAT(6(I3,F9.6))
      WRITE (8,REC=K) MAT,MMAX,ZAG,POT,RHO,MZ,WT
   20 CONTINUE
      STOP
      END
      PROGRAM EDCONV
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
C     Converts formatted electron data file FEDAT into
C     binary direct-access file UEDAT.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION NC(26),BD(26),RLOS(113)
      OPEN (7,'FEDAT')
      OPEN (8,'UEDAT',FORM='UNFORMATTED',ACCESS='DIRECT',RECL=1224)
      DO 10 K=1,100
      READ (7,*) NMAX,LKMAX
      READ (7,*) (NC(N),N=1,NMAX)
      READ (7,*) (BD(N),N=1,NMAX)
      READ (7,*) (RLOS(L),L=1,LKMAX)
      WRITE (8,REC=K) NMAX,LKMAX,NC,BD,RLOS
   10 CONTINUE
      STOP
      END
      PROGRAM PCONV
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
      DIMENSION STE(133),STN(133),RG(133),DET(133)
      DATA NMAX/133/
      OPEN (UNIT=7,FILE='FPROT')
      OPEN (UNIT=8,FILE='UPROT',FORM='UNFORMATTED',
     1 ACCESS='DIRECT',RECL=2128)
      DO 10 J=1,74
      READ (7,*) (STE(N),N=1,NMAX)
      READ (7,*) (STN(N),N=1,NMAX)
      READ (7,*) (RG(N),N=1,NMAX)
      READ (7,*) (DET(N),N=1,NMAX)
      WRITE (8,REC=J) STE,STN,RG,DET
   10 CONTINUE
      STOP
      END
      PROGRAM ACONV
C
C     8 September 1992.
C
C     Written by Martin J. Berger,
C     National Institute of Standards and Technology,
C     Gaithersburg, MD 20899.
C
      DIMENSION STE(122),STN(122),RG(122),DET(122)
      DATA NMAX/122/
      OPEN (UNIT=7,FILE='FALPH')
      OPEN (UNIT=8,FILE='UALPH',FORM='UNFORMATTED',
     1 ACCESS='DIRECT',RECL=1952)
      DO 10 J=1,74
      READ (7,*) (STE(N),N=1,NMAX)
      READ (7,*) (STN(N),N=1,NMAX)
      READ (7,*) (RG(N),N=1,NMAX)
      READ (7,*) (DET(N),N=1,NMAX)
      WRITE (8,REC=J) STE,STN,RG,DET
   10 CONTINUE
      STOP
      END
```

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Table 1. List of ID numbers and names of materials for which data are included in file UCOMP.

| | |
|---|---|
| 1 | HYDROGEN |
| 2 | HELIUM |
| 3 | LITHIUM |
| 4 | BERYLLIUM |
| 5 | BORON |
| 6 | AMORPHOUS CARBON (density 2.0 g/cm3) |
| 7 | NITROGEN |
| 8 | OXYGEN |
| 9 | FLUORINE |
| 10 | NEON |
| 11 | SODIUM |
| 12 | MAGNESIUM |
| 13 | ALUMINUM |
| 14 | SILICON |
| 15 | PHOSPHORUS |
| 16 | SULFUR |
| 17 | CHLORINE |
| 18 | ARGON |
| 19 | POTASSIUM |
| 20 | CALCIUM |
| 21 | SCANDIUM |
| 22 | TITANIUM |
| 23 | VANADIUM |
| 24 | CHROMIUM |
| 25 | MANGANESE |
| 26 | IRON |
| 27 | COBALT |
| 28 | NICKEL |
| 29 | COPPER |
| 30 | ZINC |
| 31 | GALLIUM |
| 32 | GERMANIUM |
| 33 | ARSENIC |
| 34 | SELENIUM |
| 35 | BROMINE |
| 36 | KRYPTON |
| 37 | RUBIDIUM |
| 38 | STRONTIUM |
| 39 | YTTRIUM |
| 40 | ZIRCONIUM |
| 41 | NIOBIUM |
| 42 | MOLYBDENUM |
| 43 | TECHNETIUM |
| 44 | RUTHENIUM |
| 45 | RHODIUM |
| 46 | PALLADIUM |
| 47 | SILVER |
| 48 | CADMIUM |
| 49 | INDIUM |
| 50 | TIN |
| 51 | ANTIMONY |
| 52 | TELLURIUM |
| 53 | IODINE |
| 54 | XENON |
| 55 | CESIUM |
| 56 | BARIUM |
| 57 | LANTHANUM |
| 58 | CERIUM |
| 59 | PRASEODYMIUM |
| 60 | NEODYMIUM |
| 61 | PROMETHIUM |
| 62 | SAMARIUM |
| 63 | EUROPIUM |
| 64 | GADOLINIUM |
| 65 | TERBIUM |
| 66 | DYSPROSIUM |
| 67 | HOLMIUM |
| 68 | ERBIUM |
| 69 | THULIUM |
| 70 | YTTERBIUM |
| 71 | LUTETIUM |
| 72 | HAFNIUM |
| 73 | TANTALUM |
| 74 | TUNGSTEN |
| 75 | RHENIUM |
| 76 | OSMIUM |
| 77 | IRIDIUM |
| 78 | PLATINUM |
| 79 | GOLD |
| 80 | MERCURY |
| 81 | THALLIUM |
| 82 | LEAD |
| 83 | BISMUTH |
| 84 | POLONIUM |
| 85 | ASTATINE |
| 86 | RADON |
| 87 | FRANCIUM |
| 88 | RADIUM |
| 89 | ACTINIUM |
| 90 | THORIUM |
| 91 | PROTACTINIUM |
| 92 | URANIUM |
| 93 | NEPTUNIUM |
| 94 | PLUTONIUM |
| 95 | AMERICIUM |
| 96 | CURIUM |
| 97 | BERKELIUM |
| 98 | CALIFORNIUM |
| 99 | A-150 TISSUE-EQUIVALENT PLASTIC |
| 100 | ACETONE |
| 101 | ACETYLENE |
| 102 | ADENINE |
| 103 | ADIPOSE TISSUE (ICRP) |
| 104 | AIR, DRY (NEAR SEA LEVEL) |
| 105 | ALANINE |
| 106 | ALUMINUM OXIDE |
| 107 | AMBER |
| 108 | AMMONIA |
| 109 | ANILINE |
| 110 | ANTHRACENE |
| 111 | B-100 BONE-EQUIVALENT PLASTIC |
| 112 | BAKELITE |
| 113 | BARIUM FLUORIDE |
| 114 | BARIUM SULFATE |
| 115 | BENZENE |
| 116 | BERYLLIUM OXIDE |
| 117 | BISMUTH GERMANIUM OXIDE |
| 118 | BLOOD (ICRP) |
| 119 | BONE, COMPACT (ICRU) |
| 120 | BONE, CORTICAL (ICRP) |
| 121 | BORON CARBIDE |
| 122 | BORON OXIDE |
| 123 | BRAIN (ICRP) |
| 124 | BUTANE |
| 125 | N-BUTYL ALCOHOL |
| 126 | C-552 AIR-EQUIVALENT PLASTIC |
| 127 | CADMIUM TELLURIDE |
| 128 | CADMIUM TUNGSTATE |
| 129 | CALCIUM CARBONATE |
| 130 | CALCIUM FLUORIDE |
| 131 | CALCIUM OXIDE |
| 132 | CALCIUM SULFATE |
| 133 | CALCIUM TUNGSTATE |
| 134 | CARBON DIOXIDE |
| 135 | CARBON TETRACHLORIDE |
| 136 | CELLULOSE ACETATE, CELLOPHANE |
| 137 | CELLULOSE ACETATE BUTYRATE |
| 138 | CELLULOSE NITRATE |
| 139 | CERIC SULFATE DOSIMETER SOLUTION |
| 140 | CESIUM FLUORIDE |

Table 1 (Continued)

| | |
|---|---|
| 141 | CESIUM IODIDE |
| 142 | CHLOROBENZENE |
| 143 | CHLOROFORM |
| 144 | CONCRETE, PORTLAND |
| 145 | CYCLOHEXANE |
| 146 | 1,2-DICHLOROBENZENE |
| 147 | DICHLORODIETHYL ETHER |
| 148 | 1,2-DICHLOROETHANE |
| 149 | DIETHYL ETHER |
| 150 | N,N-DIMETHYL FORMAMIDE |
| 151 | DIMETHYL SULFOXIDE |
| 152 | ETHANE |
| 153 | ETHYL ALCOHOL |
| 154 | ETHYL CELLULOSE |
| 155 | ETHYLENE |
| 156 | EYE LENS (ICRP) |
| 157 | FERRIC OXIDE |
| 158 | FERROBORIDE |
| 159 | FERROUS OXIDE |
| 160 | FERROUS SULFATE DOSIMETER SOLUTION |
| 161 | FREON-12 |
| 162 | FREON-12B2 |
| 163 | FREON-13 |
| 164 | FREON-13B1 |
| 165 | FREON-13I1 |
| 166 | GADOLINIUM OXYSULFIDE |
| 167 | GALLIUM ARSENIDE |
| 168 | GEL IN PHOTOGRAPHIC EMULSION |
| 169 | Pyrex Glass |
| 170 | GLASS, LEAD |
| 171 | GLASS, PLATE |
| 172 | GLUCOSE |
| 173 | GLUTAMINE |
| 174 | GLYCEROL |
| 175 | GUANINE |
| 176 | GYPSUM, PLASTER OF PARIS |
| 177 | N-HEPTANE |
| 178 | N-HEXANE |
| 179 | KAPTON POLYIMIDE FILM |
| 180 | LANTHANUM OXYBROMIDE |
| 181 | LANTHANUM OXYSULFIDE |
| 182 | LEAD OXIDE |
| 183 | LITHIUM AMIDE |
| 184 | LITHIUM CARBONATE |
| 185 | LITHIUM FLUORIDE |
| 186 | LITHIUM HYDRIDE |
| 187 | LITHIUM IODIDE |
| 188 | LITHIUM OXIDE |
| 189 | LITHIUM TETRABORATE |
| 190 | LUNG (ICRP) |
| 191 | M3 WAX |
| 192 | MAGNESIUM CARBONATE |
| 193 | MAGNESIUM FLUORIDE |
| 194 | MAGNESIUM OXIDE |
| 195 | MAGNESIUM TETRABORATE |
| 196 | MERCURIC IODIDE |
| 197 | METHANE |
| 198 | METHANOL |
| 199 | MIX D WAX |
| 200 | MS20 TISSUE SUBSTITUTE |
| 201 | MUSCLE, SKELETAL (ICRP) |
| 202 | MUSCLE, STRIATED (ICRU) |
| 203 | MUSCLE-EQUIVALENT LIQUID, WITH SUCROSE |
| 204 | MUSCLE-EQUIVALENT LIQUID, WITHOUT SUCROSE |
| 205 | NAPTHALENE |
| 206 | NITROBENZENE |
| 207 | NITROUS OXIDE |
| 208 | NYLON, DU PONT ELVAMIDE 8062 |
| 209 | NYLON, TYPE 6 AND TYPE 6/6 |
| 210 | NYLON, TYPE 6/10 |
| 211 | NYLON, TYPE 11 (RILSAN) |
| 212 | OCTANE, LIQUID |
| 213 | PARAFFIN WAX |
| 214 | N-PENTANE |
| 215 | PHOTOGRAPHIC EMULSION |
| 216 | PLASTIC SCINTILLATOR (VINYLTOLUENE BASED) |
| 217 | PLUTONIUM DIOXIDE |
| 218 | POLYACRYLONITRILE |
| 219 | POLYCARBONATE (MAKROLON, LEXAN) |
| 220 | POLYCHLOROSTYRENE |
| 221 | POLYETHYLENE |
| 222 | POLYETHYLENE TEREPHTHALATE (MYLAR) |
| 223 | POLYMETHYL METHACRALATE (LUCITE, PERSPEX) |
| 224 | POLYOXYMETHYLENE |
| 225 | POLYPROPYLENE |
| 226 | POLYSTYRENE |
| 227 | POLYTETRAFLUOROETHYLENE (TEFLON) |
| 228 | POLYTRIFLUOROCHLOROETHYLENE |
| 229 | POLYVINYL ACETATE |
| 230 | POLYVINYL ALCOHOL |
| 231 | POLYVINYL BUTYRAL |
| 232 | POLYVINYL CHLORIDE |
| 233 | POLYVINYLIDENE CHLORIDE, SARAN |
| 234 | POLYVINYLIDENE FLUORIDE |
| 235 | POLYVINYL PYRROLIDONE |
| 236 | POTASSIUM IODIDE |
| 237 | POTASSIUM OXIDE |
| 238 | PROPANE |
| 239 | PROPANE, LIQUID |
| 240 | N-PROPYL ALCOHOL |
| 241 | PYRIDINE |
| 242 | RUBBER, BUTYL |
| 243 | RUBBER, NATURAL |
| 244 | RUBBER, NEOPRENE |
| 245 | SILICON DIOXIDE |
| 246 | SILVER BROMIDE |
| 247 | SILVER CHLORIDE |
| 248 | SILVER HALIDES IN PHOTOGRAPHIC EMULSION |
| 249 | SILVER IODIDE |
| 250 | SKIN (ICRP) |
| 251 | SODIUM CARBONATE |
| 252 | SODIUM IODIDE |
| 253 | SODIUM MONOXIDE |
| 254 | SODIUM NITRATE |
| 255 | STILBENE |
| 256 | SUCROSE |
| 257 | TERPHENYL |
| 258 | TESTES (ICRP) |
| 259 | TETRACHLOROETHYLENE |
| 260 | THALLIUM CHLORIDE |
| 261 | TISSUE, SOFT (ICRP) |
| 262 | TISSUE, SOFT (ICRU FOUR-COMPONENT) |
| 263 | TISSUE-EQUIVALENT GAS (METHANE BASED) |
| 264 | TISSUE-EQUIVALENT GAS (PROPANE BASED) |
| 265 | TITANIUM DIOXIDE |
| 266 | TOLUENE |
| 267 | TRICHLOROETHYLENE |
| 268 | TRIETHYL PHOSPHATE |
| 269 | TUNGSTEN HEXAFLUORIDE |
| 270 | URANIUM DICARBIDE |
| 271 | URANIUM MONOCARBIDE |
| 272 | URANIUM OXIDE |
| 273 | UREA |
| 274 | VALINE |
| 275 | VITON FLUOROELASTOMER |
| 276 | WATER, LIQUID |
| 277 | WATER VAPOR |
| 278 | XYLENE |
| 906 | GRAPHITE (density 1.7 g/cm3) |

Table 2. List of ID numbers and names of materials for which codes PSTAR and ASTAR provide stopping powers and ranges.

| | |
|---|---|
| 1 | HYDROGEN |
| 2 | HELIUM |
| 4 | BERYLLIUM |
| 6 | AMORPHOUS CARBON (density 2.0 g/cm$^3$) |
| 7 | NITROGEN |
| 8 | OXYGEN |
| 10 | NEON |
| 13 | ALUMINUM |
| 14 | SILICON |
| 18 | ARGON |
| 22 | TITANIUM |
| 26 | IRON |
| 29 | COPPER |
| 32 | GERMANIUM |
| 36 | KRYPTON |
| 42 | MOLYBDENUM |
| 47 | SILVER |
| 50 | TIN |
| 54 | XENON |
| 64 | GADOLINIUM |
| 74 | TUNGSTEN |
| 78 | PLATINUM |
| 79 | GOLD |
| 82 | LEAD |
| 92 | URANIUM |
| 99 | A-150 TISSUE-EQUIVALENT PLASTIC |
| 101 | ACETYLENE |
| 103 | ADIPOSE TISSUE (ICRP) |
| 104 | AIR, DRY (NEAR SEA LEVEL) |
| 106 | ALUMINUM OXIDE |
| 111 | B-100 BONE-EQUIVALENT PLASTIC |
| 119 | BONE, COMPACT (ICRU) |
| 120 | BONE, CORTICAL (ICRP) |
| 126 | C-552 AIR-EQUIVALENT PLASTIC |
| 130 | CALCIUM FLUORIDE |
| 134 | CARBON DIOXIDE |
| 138 | CELLULOSE NITRATE |
| 139 | CERIC SULFATE DOSIMETER SOLUTION |
| 141 | CESIUM IODIDE |
| 155 | ETHYLENE |
| 160 | FERROUS SULFATE DOSIMETER SOLUTION |
| 169 | Pyrex Glass |
| 179 | KAPTON POLYIMIDE FILM |
| 185 | LITHIUM FLUORIDE |
| 189 | LITHIUM TETRABORATE |
| 191 | M3 WAX |
| 197 | METHANE |
| 200 | MS20 TISSUE SUBSTITUTE |
| 201 | MUSCLE, SKELETAL (ICRP) |
| 202 | MUSCLE, STRIATED (ICRU) |
| 203 | MUSCLE-EQUIVALENT LIQUID, WITH SUCROSE |
| 204 | MUSCLE-EQUIVALENT LIQUID, WITHOUT SUCROSE |
| 209 | NYLON, TYPE 6 AND TYPE 6/6 |
| 213 | PARAFFIN WAX |
| 215 | PHOTOGRAPHIC EMULSION |
| 216 | PLASTIC SCINTILLATOR (VINYLTOLUENE BASED) |
| 219 | POLYCARBONATE (MAKROLON, LEXAN) |
| 221 | POLYETHYLENE |
| 222 | POLYETHYLENE TEREPHTHALATE (MYLAR) |
| 223 | POLYMETHYL METHACRALATE (LUCITE, PERSPEX, PLEXIGLAS) |
| 225 | POLYPROPYLENE |
| 226 | POLYSTYRENE |
| 227 | POLYTETRAFLUOROETHYLENE (TEFLON) |
| 232 | POLYVINYL CHLORIDE |
| 238 | PROPANE |
| 245 | SILICON DIOXIDE |
| 252 | SODIUM IODIDE |
| 255 | STILBENE |
| 263 | TISSUE-EQUIVALENT GAS (METHANE BASED) |
| 264 | TISSUE-EQUIVALENT GAS (PROPANE BASED) |
| 266 | TOLUENE |
| 276 | WATER, LIQUID |
| 277 | WATER VAPOR |
| 906 | GRAPHITE (density 1.7 g/cm$^3$) |