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# ESTAR, PSTAR, ASTAR .

A PC package for calculating stopping powers and ranges of electrons, protons and helium ions

Version 2

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Abstract: A PC package is documented for calculating stopping powers and ranges of electrons, protons and helium ions in matter for energies from 1 keV up to 10 GeV. Stopping powers and ranges for electrons can be calculated for any element, compound or mixture. Stopping powers and ranges of protons and helium ions can be calculated for 74 materials (26 elements and 48 compounds and mixtures). The files are stored on two HD diskettes in compressed form. Both executable files for IBM PC and Fortran-77 source files are provided. All three programs require 5.2 Mb of diskspace. This set of two diskettes with detailed documentation is available upon request, costfree, from the IAEA Nuclear Data Section.

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

1 HYDROGEN

- 2 HELIUM 3 LITHIUM
- 3 LITHIUM 4 BERYLLIUM
- 5 BORON
- 6 AMORPHOLIS CARRON (density 2.0 m/s
- 71 LUTETIUM 72 HAFNIUM 73 TANTALUM 74 TUNGSTEN 75 RHENIUM

# ESTAR, PSTAR and ASTAR: Computer Programs for Calculating Stopping Powers and Ranges for Electrons, Protons and Helium Ions

by

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This Appendix describes three computer programs, ESTAR, PSTAR and ASTAR, which calculate stopping-powers and ranges for electrons, protons and alpha particles (helium ions). ESTAR is applicable to any element, compound or mixture. PSTAR and ASTAR are applicable to 74 materials, including many of interest in biomedical dosimetry. A detailed description of the methods used in these programs can be found in ICRU Reports 37 and 49 [1,2].

The original versions of PSTAR and ASTAR [3] are based on calculations with a fixed set of mean excitation energies from [1,2]. In Version 2 presented here, stopping powers and ranges can be adjusted so that they correspond to mean excitation energies that differ by up to 10 percent from the values used in Version 1. Furthermore, the stopping powers of graphite in version 2 of PSTAR are modified to take into account recent measurements of the amorphous-carbon/graphite stopping power ratio by Necas *et al.* [4].

The files for ESTAR, PSTAR and ASTAR are stored in compressed form in three archive files EST.EXE, PST.EXE and AST.EXE. These archives contain executable code (for use with IBM-compatible personal computers), data files, and Fortran source code. The latter can be used to compile the programs on other types of computers. The archive files are self-extracting. When used with an IBM-compatible personal computer, the commands EST, PST or AST will extract and decompress all the files from the archives.

The archive files are stored on two 3.5-inch 1.44-Mb floppy disks. Disk 1 contains EST.EXE and AST.EXE, and Disk 2 contains PST.EXE. The two disks can be obtained from the Nuclear Data Section, Division of Physical and Chemical Sciences, International Atomic Energy Agency, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, Austria.

# A.1. ESTAR: Stopping Powers and Ranges for Electrons.

### A.1.1. Output from ESTAR

ESTAR calculates the following quantities:

a) Electronic mass stopping power – average rate of energy loss per unit path length, due to Coulomb collisions that result in the ionization and excitation of atoms, MeV  $cm^2/g$ .

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		Table A.1. (Cor	tinued)	
141	CESIUM IODIDE	211	NYLON, TYPE 11 (RILSAN)	
142	CHLOROBENZENE	212	OCTANE, LIQUID	
143	CHLOROFORM	213	PARAFFIN WAX	
144	CONCRETE, PORTLAND	214	N-PENTANE	
145	CYCLOHEXANE	215	• • • • • •	

b) Radiative mass 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, MeV  $cm^2/g$ .

c) Total mass stopping power – sum of a) and b), MeV  $cm^2/g$ .

d) Density effect correction - correction term in the stopping power formula that takes into account the reduction of the electronic mass stopping power due to the polarization of the medium by the incident electron.

e) CSDA range – a 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,  $g/cm^2$ . Obtained by integrating the reciprocal of the total stopping power with respect to energy.

f) Radiation yield – fraction of the energy of primary electron converted into bremsstrahlung, calculated in the continuous-slowing-down approximation.

There are two output options:

- 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 of the tables in [1].
- Option 2 Output quantities a) through d) are tabulated at a user-selecte<sup>4</sup> set of energies between 1 keV and 10 GeV.

#### A.1.2. Method used for Electrons

Electronic mass stopping powers are calculated from the theory of Bethe [5,6], using Eq. (7.1) of Chapter 7.2, with a density-effect correction evaluated according to Sternheimer [7,8]. By default, I-values are used which are identical with those recommended in [1,2]. However, the user is given the opportunity of choosing different I-values.

The uncertainties of the calculated electronic mass stopping powers for electrons are estimated in [1] to be 1 to 2 percent above 100 keV, and 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 mainly due to the lack of shell corrections.

Radiative stopping powers are evaluated in ESTAR with a combination of theoretical bremsstrahlung cross sections described by Seltzer and Berger [9]. Analytical formulas (using high-energy approximations) are used above 50 MeV, and numerical results of Pratt *et al.* [10] below 2 MeV. Cross sections in the intermediate energy region from 2 MeV to 50 MeV are obtained by interpolation. 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.

2

Table A.2. Cutoff energies  $T_1$  and  $T_2$  used in combination of low-energy experimental and high-energy theoretical stopping powers for protons.

#### A.1.3. Required Program Files and Data Files

ESTAR can be run on an IBM-compatible personal computer, using the DOS operating system (Version 2.1 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 a binary 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 (S1 values between 0.01 and 1000 MeV).

For the installation of the program on a different type of computer, the following Fortran-77 source-code and data files (in ASCII format) are available:

ESTAR.FOR, COMPOS.FOR, EDCONV.FOR, CONVERT.FOR, FEDAT, and FCOMP.

These files are to be used as follows:

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

# A.1.4. Specification of the Properties of the Stopping Medium

ESTAR must be supplied with information about the atomic composition, density, and 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 can be read from the data file UCOMP.
- Option 2 The information for any material can be supplied from the keyboard, in response to prompts from ESTAR.

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Table A.3. Cutoff energies  $T_1$  and  $T_2$  used in combination of low-energy experimental and high-energy theoretical stopping powers for helium ions.

With both options, ESTAR provides a default I-value, which the user can accept, or replace by another value. Because of the scale y of experimental data for electrons, such a choice has to be based on a data analysis for protons or alpha particles, or on the determination of I-values from the analysis of oscillator strengths or dielectric response functions.

The UCOMP file includes data for 279 materials, which are referenced by identification (ID) numbers 1,2,...,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 other ID numbers pertain to compounds or mixtures. Table 1 gives a listing of ID numbers and names of materials. Elements appear in this list in order of increasing atomic number, and are followed by compounds and mixtures arranged alphabetically by name. The command IDLIST can be used to start a program which lists, on the monitor screen, all ID numbers and material names in UCOMP. This display can be scrolled.

Included in UCOMP are default I-values for 279 materials. The values for 25 elements and 48 compounds are identical those used in [1,2]. Those for the other compounds in UCOMP are obtained with approximate procedures adopted in [1] for materials for which direct experimental information is lacking. This involved use of a modified Bragg rule using I-values for atomic constituents that in a crude way take into account chemical-binding and phase effects (see Section 7.2.1.5).

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 ID number of the material of interest, and lists the atomic numbers and weights of the atomic constituents, the density of the material, and the I-value.

If the composition data are entered from the keyboard, 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 data for a constituent are included in the UCOMP file, it is possible (but not required) to enter the information from the UCOMP file by using the appropriate ID number. For example, for Pyrex glass (80.7% SiO<sub>2</sub>, 12.9% B<sub>2</sub>O<sub>3</sub>, 3.8% Na<sub>2</sub>O, 2.2% Al<sub>2</sub>O<sub>3</sub> and 0.4% K<sub>2</sub>O by weight) the input for Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> can be taken from UCOMP.

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Table A.4. List of ID numbers and names of materials for which codes PSTAR and ASTAR provide stopping powers and ranges.

1	HYDROGEN
2	HELIUM

139 CERIC SULFATE DOSIMETER SOLUTION

141 CESIUM IOD

ESTAR calculates, and displays on the monitor screen, the fractions by weight of the atomic constituents in a 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 the modified Bragg-additivity rule described above. The use of this procedure results in I-values that for elements are the same, and for compounds are either identical with, or 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.

# A.1.5. Specification of Electron Energies

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With Output Option 2 (see Section A.1.1) a list of energies must be supplied at which stopping powers are to be calculated. This can be done in three ways:

- a) A list of energies can be read a from default file ENG.ELE, containing 81 energies between 1 keV and 1000 MeV.
- b) A list of energies can be read from a previously prepared file. The first line of this file must contain the number of energies in the list; subsequent lines must contain the energies (in MeV), separated by blanks.
- c) The desired list of energies can be entered from the keyboard, in response to prompts from ESTAR.

In cases b) and c), ESTAR issues a warning if at least one of the requested energies is smaller than 10 keV. ESTAR halts if it encounters an energy below 1 keV.

#### A.2. PSTAR and ASTAR: Stopping Powers and Ranges for Protons and Helium Ions

#### A.2.1. Output from PSTAR and ASTAR

The following quantities are calculated:

- a) Electronic mass stopping power average rate of energy loss per unit path length, due to Coulomb collisions that result in the ionization and excitation of atoms, MeV cm<sup>2</sup>/g.
- b) Nuclear mass stopping power average rate of energy loss per unit path length, due to elastic Coulomb collisions with atomic nuclei, MeV  $cm^2/g$ .
- c) Total mass stopping power sum of a) and b), MeV cm<sup>2</sup>/g.

- d) CSDA range an extremely close approximation to the average path length traveled by a charged particle as it slows down to rest, in g/cm<sup>2</sup>, calculated in the continuousslowing-down approximation. Obtained by integrating the reciprocal of the total stopping power with respect to energy.
- e) Projected range average value of the depth to which a charged particle penetrates in the course of slowing down to rest, in MeV  $cm^2/g$ . This depth is measured along the initial direction of the particle.
- f) Detour factor ratio of the projected range to the CSDA range (always smaller than unity, due to multiple-scattering detours)

# A.2.2. Method of Calculation for Protons and Helium Ions

PSTAR and ASTAR rely on interpolation in a database of stopping powers and ranges. A brief description will now be given of the methods used for producing this database.

A.2.2.1. Merger of High-Energy Theory and Low-Energy Data. Electronic mass stopping powers are evaluated from Bethe's theory at high energies, and from experimentallybased fitting formulas at low energies. 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 a cubic spline. Actually the cubic-spline fit is made for the quantity  $\beta^2(S/\rho)$ , where  $\beta$  is the particle speed in units of the speed of light, and  $S/\rho$  is the mass stopping power. The cubic-spline function is used to obtain, by interpolation, stopping powers at energies between  $T_1$  and  $T_2$ . The values of  $T_1$  and  $T_2$  are adjusted individually for each material to obtain a visually pleasing plot of stopping power vs. energy. The adopted values of  $T_1$  and  $T_2$ are given in Table 2 for protons, and in Table 3 for helium ions.

The uncertainties of the electronic mass stopping powers in the high-energy region are estimated to be 1 to 2 percent for elements, and 1 to 4 percent for compounds. The uncertainties in the low-energy region 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.

A.2.2.2 Stopping Power Theory at High Energies. Stopping powers are calculated according to the formulas given in Chapter 7.3.1.1.\* The shell corrections for most elements are based on semi-empirical formulas developed by Bichsel (described in [1]). For most materials the shell corrections, together with the default I-values, are those denoted as "Model 1" in [2].

This was done with a program BEST, which combines codes from ESTAR for the calculation of the density effect correction with subroutines for the calculation of the Bloch, Barkas and shell corrections from an unpublished program of H. Bichsel. With BEST one can obtain stopping powers for stripped particles of any mass or charge.

For elements with atomic numbers Z = 47, 64, 74, 78, 79, 82 and 92 two sets of calculations are made, one with shell corrections from Model 1, and another with shell corrections and I-values from a Model 2 due to Bichsel [11]. The calculations with Model 2 are used up to an energy  $T_3$ , and those with Model 1 above energy  $T_4$ , and stopping-power values between  $T_3$  and  $T_4$  are obtained by cubic-spline interpolation. The values of  $T_3$  and  $T_4$  are taken to be 25 MeV and 100 MeV for protons, and 100 MeV and 400 MeV for helium ions.

The Barkas correction is calculated according to the method of Ashley *et al.* [12,13], with parameter values used in [1]. For elements with atomic numbers Z = 47, 64, 74, 78, 79, 82 and 92, empirical Barkas correction from [14] are used. The density-effect correction is evaluated according to Sternheimer [7,3], and is significant only for protons with energies of several hundred MeV or higher.

A.2.2.3. Adjustment of Mean Excitation Energy. For each material ESTAR calculates the stopping powers in the high-energy region three times, with different I-values: with the default value (from [1,2]) and with values that are 10 percent lower, and 10 percent higher, than the default value. The results from these three calculations are merged with the same set of fitted low-energy stopping powers. Stopping powers with intermediate I-values can be accurately calculated by interpolation with respect to logI.

For elements with atomic numbers Z = 47, 64,74, 78, 79, 82 and 92, the Bethe formula with Model-2 shell corrections quite accurately represents a large body of experimental data in the energy region from 0.3 MeV to 20 MeV [11]. For these elements the changes of the stopping power due to differences of the I-value from the default value are therefore only evaluated for protons above 25 MeV and helium ions above 100 MeV.

In view of the differences between the I-values recommended by various authors (see, e.g., the discussion in Chapter 7.2.1), the opportunity of varying the I-values in ESTAR is useful, but should be used with care. One should keep in mind that many of the default I-values adopted in [1,2] are obtained in an analysis of measured stopping powers or ranges that involved the simultaneous determination of I-values and of various parameters pertaining to the shell corrections and Barkas corrections. A change of an I-value may therefore require a corresponding adjustment of these corrections, to ensure that the calculated and experimental stopping powers remain in adequate agreement. References to the available experimental literature for such an analysis can be found in the bibliographies of Andersen [15] and Powers [16].

A.2.2.4 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 [17] with numerical coefficients adopted in [2], which - except for a few materials - are from Andersen and Ziegler [18] for protons, and from Ziegler [19] or Watt [20] for alpha particles. For a few materials use is made of a different fitting formula for alpha-particle stopping powers developed by Powers [21].

For compounds for which no experimental stopping power data are available, the Bragg additivity rule is used, and mass stopping powers are 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.

**A.2.2.5.** 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 *et al.* [22]. For protons the screened potential is assumed to be the Thomas-Fermi potential as parameterized by Molière [23]. For alpha particles, the "universal" ion-atom potential of Ziegler *et al.* [24] 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 [2] 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.

A.2.2.6 CSDA and Projected Ranges. CSDA ranges are calculated by integrating the reciprocal of the total stopping power (electronic plus nuclear) with respect to energy. Projected ranges are obtained in a transport calculation according to the method of Lewis [25], which uses the elastic scattering cross sections mentioned above.

#### A.2.3. Required Program and Data Files\*

PSTAR and ASTAR can be run on an IBM-compatible personal computer using the DOS operating system (Version 2.1 or higher). A mathematical coprocessor is required. The following files are required to run PSTAR:

PSTAR.EXE	executable code for generating a stopping-power and range table
UPROT0	database that contains stopping power and range data calculated with default I-values
UPROTL	similar to UPROT, but calculated with I values 10 percent smaller than the default I-values
UPROTH	similar to UPROT, but calculated with I-values 10 percent larger than the default I-values
NAMES	set of names of the 74 materials in the database

The files FCOMP, UCOMP, COMPOS.EXE, COMPOS.FOR and CONVERT.FOR are used in ESTAR as well as PSTAR and ASTAR. However, PSTAR and ASTAR use only part of the information stored in FCOMP and UCOM.

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 required to run ASTAR:

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ASTAR.EXE	executable code for generating a stopping-power and range table
UALPH0	database that contains stopping power and range data
UALPHL	similar to UPROT, but calculated with I-values 10 percent smaller than the default I-values
UALPHH	similar to UPROT, but calculated with I-values 10 percent larger than the default I-values
NAMES	set of names of the 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.

For the installation of the program on a different type of computer, the following Fortran-77 source-code and data files (in ASCII format) are available:

For Protons:	For Helium lons:	For Both:
PSTAR.FOR	ASTAR.FOR	COMPOS.FOR
PCONVERT.FOR	ACONVERT.FOR	CONVERT.FOR
FPROT	FALPH	FCOMP
FPROTL	FALPHL	
FPROTH	FALPHH	

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These files are to be used as follows:

- a) PSTAR.FOR, ASTAR.FOR, PCONVERT.FOR, ACONVERT.FOR and CONVERT.FOR must be compiled individually to generate executable code
- b) PCONVERT must be run, using formatted files FPROT0, FPROTL or FPROT1 as input, to generate unformatted direct-access files UPRPOT0, UPROTL or UPROTH
- c) ACONVERT must be run, using formatted files FALPH0, FALPHL or FALPHH as input, to generate unformatted direct-access files UALPH0, UALPHL or UALPHH
- d) CONVERT must be run, using formatted file FCOMP as input, to generate unformatted direct-access file UCOMP.

# A.2.4. 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 4 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 of the material
- c) The mean excitation energy of the material

# A.2.5. Specification of Energies

A list of energies must be supplied at which stopping powers are to be calculated. This can be done in three ways:

- a) A list of energies can be read from a default file ENG.PRO for protons (133 energies between 1 keV and 10,000 MeV) or from a default file ENG.ALF for helium ions (122 energies between 1 keV and 1000 MeV).
- b) A list of energies can be read from a previously prepared file. The first line of this file must contain the number of energies in the list; subsequent lines must contain the energies (in MeV), separated by blanks.
- c) The desired list of energies-can be entered from the keyboard, in response to prompts from PSTAR or ASTAR.

#### A.2.6. Choice of Mean Excitation Energy

PSTAR and ASTAR display on the monitor screen the default I-value of the material, and prompt the user to indicate whether this value is acceptable. If the reply is negative, the program displays the three I-values for which stopping powers are available for interpolation: the default value  $I_{def}$ ,  $I_1 = I_{def}/1.1$  and  $I_2 = 1.1 I_{def}$ . The user is then asked to specify the desired I-value,  $I_2$ . When making this choice, the user should keep in mind the cautionary remarks in Section A.2.2.4.

If  $I_s$  lies between  $I_1$  and  $I_2$ , the program uses quadratic polynomial interpolation with respect to logI to determine the stopping power. If  $I_s$  is smaller than  $I_1$  or larger than  $I_2$ , the program uses linear extrapolation with respect to logI. Extrapolation should of course be used with caution.

#### REFERENCES

- [1] International Commission on Radiation Units and Measurements, ICRU Report 37, Stopping Powers for Electrons and Positrons, 1984.
- [2] International Commission on Radiation Units and Measurements, ICRU Report 49, Stopping Powers and Ranges for Protons and Alpha Particles, 1993.
- [3] M. J. Berger, ESTAR, PSTAR and ASTAR: Computer Codes for Calculating Stopping Power and Range Tables for Electrons, Protons and Helium Ions, National Institute of Standards and Technology Report NISTIR 4999, 1992.
- [4] V. Necas, W. Käferbock, W. Rossler and P. Bauer, Nucl. Inst. Meth. B, in press.
- [5] H. Bethe, Ann. d. Physik 5, 325, 1930.
- [6] H. Bethe, Z. Phys. 76, 293, 1932.
- [7] R. M. Sternheimer, Phys.Rev. 88, 851, 1952.
- [8] R. M. Sternheimer, S. M. Seltzer, and M. J. Berger, Phys. Rev. B. 26, 6067, 1982.
- [9] S. M. Seitzer and M. J. Berger, Nucl. Instr. Meth. B12, 95, 1985.
- [10] R. H. Pratt, H. K. Tseng, C. M. Lee, L. Kissel, C. MacCallum, and M. Riley, Atomic Data Nucl. Data Tables 20, 175, 1977. Errata in 26, 477, 1981.
- [11] H. Bichsel, Phys. Rev. A, 46, 5761, 1992.
- [12] J. C. Ashley, R. H. Ritchie and W. Brandt, Phys. Rev. B, 5, 2393, 1972.
- [13] J. C. Ashley, R. H. Ritchie and W. Brandt, Phys. Rev. A, 8, 2402, 1973.
- [14] H. Bichsel, Phys. Rev. A, 41, 3642, 1990.
- [15] H. H. Andersen, Bibliography and Index of Experimental Stopping Power and Range Data, Pergamon Press (Elmsford, N.Y.), 1977.
- [16] D. Powers, Topical Survey of the Literature on Experimental and Theoretical Stopping
   Power Phenomena for Energetic Protons, Helium Ions, and Heavy Ions in Matter for the Period 1977-1987, Internal Report, Department of Physics, Baylor University, Waco, Texas, 1988.
- [17] C. Varelas and J. Biersack, Nucl. Instr. Meth. 79, 213, 1970.
- [18] H. H. Andersen and J. F. Ziegler, Hydrogen: Stopping Powers and Ranges in All Elements, Pergamon Press (Elmsford, N.Y.), 1977.

- [19] J. F. Ziegler, *Helium: Stopping Powers and Ranges in All Elemental Matter*, Pergamon Press (Elmsford, N.Y.), 1977.
- [20] D. E. Watt, Stopping Cross Sections, Mass Stopping Powers and Ranges in 30 Elements for Alpha Particles (1 keV to 100 MeV), Internal Report, Department of Physics and Astronomy, University of St. Andrews, Scotland, 1988.
- [21] D. Powers, Stopping Cross Sections and Ranges of Alpha Particles in Matter, Internal Report, Department of Physics, Baylor University, Waco, Texas, 1977.
- [22] E. Everhart, G. Stone, and R. J. Carbone, Phys. Rev. 99, 1287, 1955.
- [23] G. Molière, Z. f. Naturf. 2a, 133, 1947.

- .

- [24] J. F. Ziegler, J. P. Biersack and U. Littmark, *The Stopping and Range of Ions in Solids*, Pergamon Press (Elmsford, N.Y.), 1985.
- [25] H. W. Lewis, Phys. Rev. 78, 526, 1950.

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

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1	HYDROGEN	71	LUTETIUM
2 3	HELIUM	72	HAFNIUM
4	LIT HIUM BERYLLIUM	73 74	TANTALUM TUNGSTEN
5	BORON	74	RHENIUM
6	AMORPHOUS CARBON (density 2.0 g/cm <sup>3</sup> )	76	OSMIUM
7	NITROGEN	77	RIDIUM
8	OXYGEN	78	PLATINUM
9	FLUORINE	79	GOLD
10	NEON	80	MERCURY
11	SODIUM	81	THALLIUM
12	MAGNESIUM	82	LEAD
13	ALUMINUM	83	BISMUTH
14	SILICON	84	POLONIUM
15	PHOSPHORUS	85	ASTATINE
16	SULFUR	86	RADON
17	CHLORINE	87	FRANCIUM
18	ARGON	88	RADIUM
19	POTASSIUM	89	ACTINIUM
20 21	CALCIUM	90	THORIUM
22	SCANDIUM TITANIUM	91 92	PROTACTINIUM
23	VANADIUM	92	URANIUM NEPTUNIUM
24	CHROMIUM	93	
25	MANGANESE	95	AMERICIUM
26	IRON	96	CURIUM
27	COBALT	97	
28	NICKEL	98	
29	COPPER	99	
30	ZINC	100	-
31	GALLIUM	101	ACETYLENE
32	GERMANIUM	102	ADENINE
33		103	ADIPOSE TISSUE (ICRP)
34		104	AIR, DRY (NEAR SEA LEVEL)
35			ALANINE
36			ALUMINUM OXIDE
37			AMBER
38			AMMONIA
39			ANILINE
40 41			ANTHRACENE
42			B-100 BONE-EQUIVALENT PLASTIC BAKELITE
43			BARIUM FLUORIDE
44			4 BARIUM SULFATE
45			5 BENZENE
46			6 BERYLLIUM OXIDE
47			7 BISMUTH GERMANIUM OXIDE
48			8 BLOOD (ICRP)
49			9 BONE, COMPACT (ICRU)
50			0 BONE, CORTICAL (ICRP)
51	ANTIMONY	12	1 BORON CARBIDE
52	TELLURIUM	12	2 BORON OXIDE
5:	3 IODINE	12	3 BRAIN (ICRP)
54	XENON	12	4 BUTANE
5:		12	S N-BUTYL ALCOHOL
5		12	6 C-552 AIR-EQUIVALENT PLASTIC
5			7 CADMIUM TELLURIDE
5			CADMIUM TUNGSTATE
	PRASEODYMIUM		29 CALCIUM CARBONATE
			CALCIUM FLUORIDE
	1 PROMETHIUM		CALCIUM OXIDE
	2 SAMARIUM 3 EUROPIUM		2 CALCIUM SULFATE
	3 EUROPIUM 4 GADOLINIUM		33 CALCIUM TUNGSTATE 34 CARBON DIOXIDE
	5 TERBIUM	-	34 CARBON DIOXIDE 35 CARBON TETRACHLORIDE
	6 DYSPROSIUM -		36 CELLULOSE ACETATE, CELLOPHANE
	7 HOLMIUM		37 CELLULOSE ACETATE BUTYRATE
	8 ERBIUM		38 CELLULOSE NITRATE
	9 THULIUM		39 CERIC SULFATE DOSIMETER SOLUTION
	0 YTTERBIUM		40 CESIUM FLUORIDE
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#### Table A.1. (Continued)

	1 able A.1
141 CESIUM IODIDE 142 CHLOROBENZENE	
143 CHLOROFORM	
144 CONCRETE, PORTLAND	
145 CYCLOHEXANE	
146 1,2-DICHLOROBENZENE	
14/ DICHLORODIETHYLETHER	
148 1,2-DICHLOROETHANE	
149 DIETHYL ETHER	
150 N,N-DIMETHYL FORMAMIDE	
151 DIMETHYL SULFOXIDE 152 ETHANE	
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 SOLUT	MON
161 FREON-12	
162 FREON-12B2 163 FREON-13	
163 FREON-13 164 FREON-13B1	
165 FREON-1311	
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	
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	
197 METHANE 198 METHANOL	
199 MIX D WAX	
200 MS20 TISSUE SUBSTITUTE	
201 MUSCLE, SKELETAL (ICRP)	
202 MUSCLE, STRIATED (ICRU)	
203 MUSCLE-EQUIVALENTLIQUID, WITH	SUCROSE
204 MUSCLE-EQUIVALENT LIQUID, WITH	IOUT SUCRO
205 NAPTHALENE	
206 NITROBENZENE	
207 NITROUS OXIDE 208 NYLON, DU PONT ELVAMIDE 8062	
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 PARAFFIN WAX 213 214 N-PENTANE PHOTOGRAPHIC EMULSION 215 PLASTIC SCINTILLATOR (VINYLTOLUENE BASED) 216 PLUTONIUM DIOXIDE 217 POLYACRYLONITRILE 218 POLYCARBONATE (MAKROLON, LEXAN) 219 POLYCHLOROSTYRENE 220 221 POLYETHYLENE POLYETHYLENE TEREPHTHALATE (MYLAR) 222 223 POLYMETHYL METHACRALATE (LUCITE, PERSPEX) 224 POLYOXYMETHYLENE 225 POLYPROPYLENE 226 POLYSTYRENE **POLYTETRAFLUOROETHYLENE(TEFLON)** 227 228 POLYTRIFLUOROCHLOROETHYLENE 229 POLYVINYL ACETATE 230 POLYVINYL ALCOHOL 231 BUTYRAL POLYVINYL CHLORIDE 232 POLYVINYLIDENECHLORIDE, SARAN 233 234 **POLYVINYLIDENE FLUORIDE** 235 POLYVINYL PYRROLIDONE POTASSIUM IODIDE 236 237 POTASSIUM OXIDE 238 PROPANE PROPANE, LIQUID 239 240 N-PROPYL ALCOHOL 241 PYRIDINE RUBBER, BUTYL 242 243 RUBBER, NATURAL RUBBER, NEOPRENE 244 245 SILICON DIOXIDE 246 SILVER BROMIDE 247 SILVER CHLORIDE SILVER HALIDES IN PHOTOGRAPHIC EMULSION 248 SILVER IODIDE 249 SKIN (ICRP) 250 SODIUM CARBONATE 251 SODIUM IODIDE 252 SODIUM MONOXIDE 253 254 SODIUM NITRATE 255 STILBENE 256 SUCROSE 257 TERPHENYL TESTES (ICRP) 258 TETRACHLOROETHYLENE 259 THALLIUM CHLORIDE 260 261 TISSUE, SOFT (ICRP) 262 TISSUE, SOFT (ICRU FOUR-COMPONENT) 263 TISSUE-EQUIVALENT GAS (METHANET SED) TISSUE-EQUIVALENT GAS (PROPANE BASED) 264 265 TITANIUM DIOXIDE TOLUENE 266 TRICHLOROETHYLENE 267 TRIETHYL PHOSPHATE 268 TUNGSTEN HEXAFLUORIDE 269 270 URANIUM DICARBIDE 271 URANIUM MONOCARBIDE URANIUM OXIDE 272 UREA 273 VALINE SE 274 VITON FLUOROELASTOMER 275

- 276 WATER, LIQUID
- 277 WATER VAPOR
- 278 XYLENE
- 906 GRAPHITE (density 1 7 g/cm3)

ID No.	T <sub>1</sub> (MeV)	T <sub>2</sub> (MeV)	ID No.	T <sub>1</sub> (MeV)	T <sub>2</sub> (MeV)
1	0.2	0.5	134	0.2	0.5
	0.25	0.5	138	0.3	0.5
2 4 6	0.3	0.5	139	0.2	0.5
	0.2	0.5	141	<b>0.8</b> ·	2.0
7,8	0.25	0.5	155,160,169	0.2	0.5
10,13	<b>`0.3</b>	1.0	179	0.3	0.5
14	0.5	0.8	185,189	0.2	0.5
18	0.5	1.0	191	0.2	- 0.5
22	0.5	1.5	197	0.2	0.5
26,29	0.5	1.0	200	0.3	0.5
32,36	0.5	1.5	201,202,203,204	0.2	0.5
42,47	0.75	2.0	209,213	0.3	0.5
50	0.5	1.5	215	0.8	3.0
54,64	0.5	1.0	216,219,221,222	0.3	0.5
74,78 79	0.3	0.5	223	0.2	0.5
82	0.5	1.0	225,226	0.3	0.5
92	0.25	1.0	227,232,238	0.2	0.5
99	0.5	1.0	245	0.3	0.5
101	0.2	0.5	252	0.8	3.0
103	0.3	0.5	255	0.2	0.5
104,106	0.2	0.5	263,264,266	0.3	0.5
111,119,120	0.3	0.5	276	0.15	0.5
126	0.2	0.5	277	0.3	0.5
130	0.3	0.5			

Table A.2. Cutoff energies  $T_1$  and  $T_2$  used in combination of low-energy experimental and high-energy theoretical stopping powers for protons.

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ID No.	T <sub>1</sub> (MeV)	T <sub>2</sub> (MeV)
1	1.0	2.0
2	1.5	3.0
4	1.0	4.0
6	1.0	3.0
7,8,10	1.0	2.0
13,14	2.0	4.0
18	0.8	3.0
22,26,29,32	2.0	6.0
36	3.0	7.0
42,47,50,54	2.0	5.0
64,74,78	1.0	3.0
79,82	1.0	2.0
92	1.0	4.0
99	1.0	2.0
101	1.0	3.0
103	0.8	2.0
104,106,111,119,120	1.0	2.0
126,130,134,138,139	1.0	3.0
141	1.0	5.0
155,160,159,179	1.0	2.0
185	1.0	3.0
189	0.8	2.0
191	1.0	2.0
197	0.6	2.0
200,201,202,203,204,209,213	1.0	2.0
215	0.6	5.0
216,219,221,222,223,225,226,227	1.0	2.0
232	1.0	4.0
238,245,252	1.0	2.0
255	1.0	3.0
263.264,266,276,277	1.0	2.0

Table A.3. Cutoff energies  $T_1$  and  $T_2$  used in combination of low-energy experimental and high-energy theoretical stopping powers for helium ions.

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Table A.4. 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
- AMORPHOUS CARBON (density 2.0 g/cm<sup>3</sup>) 6
- 7 NITROGEN
- 8 OXYGEN
- 10 NEON
- 13 ALUMINUM
- 14 SILICON
- 18 ARGON
- 22 **TTANIUM**
- 26 IRON
- COPPER 29
- 32 GERMANIUM
- 36 KRYPTON
- 42 MOLYBDENUM
- 47 SILVER
- 50 "TIN
- 54 XENON
- 64 GADOLINIUM
- 74 TUNGSTEN
- 78 PLATINUM
- GOLD 79
- 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 (ICRF)
  - 202 MUSCLE, STRIATED (ICRU)
  - 203 MUSCLE-EQUIVALENTLIQUID, WITH SUCROSE
  - 204 MUSCLE-EQUIVALENTLIQUID, 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 POLYETHYLENETEREPHTHALATE (MYLAR)
  - 223 POLYMETHYL METHACRALATE (LUCITE, PERSPEX, PLEXIGLAS)

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- 225 POLYPROPYLENE
- 226 POLYSTYRENE
- 227 POLYTETRAFLUOROETHYLENE(TEFLON)
- 232 POLYVINYL CHLORIDE
- 238 PROPANE
- 252 SODIUM IODIDE
- 255 STILBENE
- TISSUE-EQUIVALENT GAS (METHANE BASED)
- 276 WATER, LIQUID
- 277 WATER VAPOR
- 906 GRAPHITE (density 1.7 g/cm<sup>3</sup>)

- 245 SILICON DIOXIDE

- 263
   TISSUE-EQUIVALENT GAS (METHANE BASED)

   264
   TISSUE-EQUIVALENT GAS (PROPANE BASED)
- 266 TOLUENE