



2. ESTAR: Stopping Powers and Ranges for Electrons

Access the **ESTAR** Database

2.1. Overview

There are two ways to use the ESTAR database. The full-featured version gives the user many capabilities (i.e., file uploading, graphing, and formatted tables). The text-based version only outputs a basic text table of data. This may be useful if the data are to be exported to the user's speadsheet program.

2.2. Output of ESTAR

The following quantities are calculated:

- a Collision stopping power, MeV cm²/g;
- b Radiative stopping power, MeV cm²/g;
- c Total stopping power (sum of a and b), MeV cm²/g;
- d Density effect parameter "delta";
- e CSDA (continuous-slowing-down approximation) range, g/cm²;
- f Radiation yield (fraction of kinetic energy of primary electron converted into bremsstrahlung).

The significance of these quantities is briefly indicated in the <u>Appendix</u>.

The graphical version of the database also has the ability to graph the calculated data. Next to the image are buttons that allow you to resize the image which may be useful if you are printing.

2.3. Stopping Medium

ESTAR must be supplied with information about the atomic composition, the density, and the mean excitation energy (I-value) of the material. You may either 1) use a list of common materials which run with preset composition data; or 2) define the composition of a unique material.

- 1) <u>Table 1</u> is a list of the over 250 **common materials** available. The first items listed are <u>elements</u> ordered by atomic number. These are followed by <u>compounds and mixtures</u> listed alphabetically. You can display the <u>compositional data</u> (atomic constituents, density at 20 °C, 101 325 Pa (1 atm), and mean excitation energy) of these common materials (also available in a <u>text-only [table-free] version</u>). (Note: on the Macintosh platform, with versions of Netscape Navigator earlier than version 4.0, only the first 254 materials can be selected.)
- 2) There are three required fields to specify a unique material:
 - a Name
 - b Density in grams per cubic centimeter
 - c Atomic constituents

For the atomic constituents entry: Each line should have an element or compound followed by a space and then the fraction by weight. Weight fractions that do not equal unity will be normalized. Only elements 1 through 98 are available. Chemical

formulas for compounds should be entered in standard chemical notation, with appropriate upper and lower case. However, because of hardware limitations, subscripts must be written on the line (i.e., calcium tungstate must be entered as CaWO4). Parentheses, spaces and dots may not be used (i.e., calcium phosphate must be entered as Ca3P2O8 and not as Ca3(PO4)2). Substances consisting of molecules with only a single species of atoms can be designated as either elements or compounds. For example, molecular nitrogen could be treated as an element with symbol N, or as a compound with formula N2.

ESTAR will provide a default I-value for any unique 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 for the common materials. This value may be changed by the user.

Warning: Unrealistic input can result in unpredictable output (i.e., a broken image and/or NaNQ printed in the data table).

2.4. Energy List

ESTAR may be run with a list of 80 - 100 default energies (10 keV to 1 GeV) or with user-defined energies (1 keV to 10 GeV). *Note:* ESTAR will not calculate range or yield information when user-defined energies are used. Additional energies may be merged into the default list or the defaults can be excluded. There are two options for entering additional energies:

1) File uploading: (You must have a file upload compatible browser) Energy values should be entered in MeV and separated by Return or Enter. The file should be in ASCII format containing one additional energy per line.

Example:

0.01

1.23

2.03E3

5E-3

100.23

2) Manual input: A text box is provided for manual entry of additional energies. This is the only method available for browsers that do not handle file uploading. One should be able to copy and paste the energy values into this box. The format is one energy per line as above.

Warning: At low energies the accuracy of stopping powers may be poor. See below.

2.5. Method

Collision stopping powers are calculated from the theory of <u>Bethe</u> (1930, 1932), with a density-effect correction evaluated according to <u>Sternheimer</u> (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 (<u>ICRU, 1984</u>). 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 (ICRU, 1984) to be 1 % to 2 % above 100 keV, 2 % to 3 % (in low-Z materials) and 5 % to 10 % (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. 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 to the order of 10 % at 1 keV. ESTAR will not run below 1 keV.

Radiative stopping powers are evaluated in ESTAR with a combination of theoretical bremsstrahlung cross sections described by <u>Seltzer and Berger</u> (1985). Analytical formulas (using a high-energy approximation) are used above 50 MeV,

and accurate numerical results of <u>Pratt et al</u>. (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 % above 50 MeV, 2 % to 5 % between 50 MeV and 2 MeV, and 5 % below 2 MeV.

ESTAR Database



Text Version

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