NIST

NIST Electron and Positron Stopping Powers of Materials Database
Version 2.0

Users' Guide

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National Institute of Standards and Technology
Standard Reference Data Program
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ACKNOWLEDGEMENTS

CONTENTS

INTRODUCTION

This database contains data related to the electron and positron stopping powers of various materials. The database calculates collision, radiative, and total stopping powers, CSDA ranges and radiation (bremsstralung) yields for electrons or positrons with kinetic energies from 1 keV to 10 GeV.

The methods used give results consistent with those in NBSIR 82-2550-A, "Stopping Powers and Ranges of Electrons and Positrons (2nd Ed.), M.J. Berger and S.M. Seltzer (1983), and in ICRU Report 37, "Stopping Powers for Electrons and Positrons" (1984). This version of EPSTAR incorporates updated radiative energy-loss data given by S.M. Seltzer and M.J. Berger, Nucl. Instrum. Methods B12, 95 (1985) and Atomic Data and Nuclear Data Tables 35, 345 (1986), and in L. Kim, R.H. Pratt, S.M. Seltzer and M.J. Berger, Phys. Rev. A 33, 3002 (1986).

It is recommended that the user be familiar with either ICRU Report 37 or NBSIR 82-2550-A, particularly in regard to the determination of the mean excitation energy and the density-effect correction used in the Bethe formula for the collision stopping power.

USE OF THE DATABASE

The database is accessed by an interactive program that allows the user to specify the energy list, the incident particle (electron or positron), and the target density. If the target is a gas, the temperature and pressure for the specified density and those at which the calculation is to be made, are entered. The target material is defined in terms of relative parts either by weight or by number (partial pressures for gases). Target material constituents are entered in terms of chemical formulas using standard chemical symbols. (This input is case-sensitive; i.e., for calcium, use Ca, not CA or ca.) The input is summarized, and an opportunity is given to add constituents to the defined target. Once the target composition is accepted, the program calculates a mean excitation energy (I-value) for which an override option is available. Appendix B gives experimentally derived I-values for selected materials. Finally, the material is characterized as an insulator or conductor for the calculation of the density-effect correction, but an option to change this designation is also available. From this input, the quantities listed above are calculated and appear on the screen. The results may be saved to a file. Example runs are shown in Appendix A.

Help is available at most prompts by entering a question mark. The help screens are reproduced in Appendix C. It may be useful to read through Appendix C before using the database.

EPSTAR 1

SYSTEM REQUIREMENTS

MS-DOS or PC-DOS computer with DOS 2.1 or later version
Memory 256 kbytes
Math coprocessor
CONFIG.SYS file must contain "DEVICE = ANSI.SYS"
ANSI.SYS must be in your root directory
Hard disk with 320 kbytes (optional)

Distribution is available on:

5¼" (1.2 Mbytes) diskette
5¼" (360 kbytes) diskette
3½" (720 kbytes) diskette

INSTALLATION

The database may be run from the diskette by changing to your diskette drive (ex: A:) and typing EPSTAR. The database may be run from your hard drive. Copy the files on the diskette to your hard drive. For example, to store the files in a subdirectory called EPSTAR:

1.	Change to the hard drive	**C:**
2.	Make a subdirectory	**MD EPSTAR**
3.	Change to that subdirectory	**CD EPSTAR**
4.	Copy the files from diskette	**COPY A:*.***

When you run the program, change to the subdirectory where you copied the files (CD EPSTAR in the above example), and type EPSTAR to execute the program.

The files on the diskette are:

EPSTAR.EXE – the program

BINDENGY.BIN
PHIRADB.BIN } the data files
POSRATB.BIN

EPSTR001.HLP
. . .   .HLP } the data files
EPSTR025.HLP

EPSTAR 2

Appendix A

EXAMPLE RUNS

Two examples are included: The first is a simple material (CH4), the second is a complex material (pyrex glass). User responses are shown in **boldface** *type.*

*1. Start the program: a. Change to the directory where the program
is located.
EX* **a:**
to change drive, or
    c:\dirname
to change directory

*b. Type the program name followed by the
enter key:* **epstar** *<cr>*

The following copyright screen will appear:

```
                    NIST Standard Reference Database 7

       NIST ELECTRON AND POSITRON STOPPING POWERS AND RANGES
                               DATABASE
                              Version 2.0

                              Written by
                          STEPHEN M. SELTZER
                       Center for Radiation Research
                 National Institute of Standards and Technology
                          Gaithersburg, MD 20899

                             Distributed by
                        Standard Reference Data
                 National Institute of Standards and Technology
                          Gaithersburg, MD 20899

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                 on behalf of the United States Government

    Help (Y/N)? N
```

2. Copies of the detailed help screens are available in Appendix C.

For an overview of the program, enter Y <cr>; or as in this example, enter <cr> to start the program.

EPSTAR 3

EXAMPLE 1

```
                                                        X to Exit
   Kinetic energy list options:
       1. Take default energy list (extends from 1 keV to 10 GeV).
       2. Input own energy list.
   Selection (1/2)? 2
```

Selection of item 2 requires entry of specific energies as follows:

```
   A blank entry ends the list.

   Enter value for energy # 1 in MeV: .1

   Enter value for energy # 2 in MeV: 1.

   Enter value for energy # 3 in MeV: 10.

   Enter value for energy # 4 in MeV:
```

The blank entry ended the list.

```
                                                        X to Exit
   Select electrons or positrons (-/+): -

   Enter name of material:   Methane
   (used in table heading)

   Enter density (g/cm3) of material: 7.168E-04

   Enter temperature (°C) for which density is specified: 0

   Enter pressure (atm) for which density is specified: 1.

   Enter temperature (°C) for which calculation is to be done: 20

   Enter pressure (atm) for which calculation is to be done: 1.
```

Once the parameters are set, specify the target material.

Override I-values can be included for each constituent (? for help).

```
   Abundances for constituents of the material can be input as:
       1. Relative parts by weight.
       2. Relative parts by number (partial pressures for gases).
   Selection (1/2)? 2
```

EPSTAR 4

```
                                                        X to Exit
    A blank entry ends the list.

    An override I-value can be included
    for each constituent (? for help).

    Enter chemical formula for constituent # 1: CH4

    Enter relative abundance for constituent # 1: 100

    Enter chemical formula for constituent # 2:

```

When all information is entered, the program summarizes the defined materials and allows changes.

```
                                                        X to Exit
    Input Summary:

        #    Abundance   Formula
        1    100.00000   CH4
    Total    100.00000

    Add constituents (Y/N)? N

```

```
                                                        X to Exit

    Based on your input, the mean excitation energy (I-value) for the material
    has been calculated to be 41.7 eV. You can:
         1. Accept this value.
         2. Enter another value.
         3. Consult a list of experimentally-derived values for some materials.
    Selection (1/2/3)? 1

    In the calculation of the density-effect correction to the collision stopping
    power, the atomic electrons in the outermost shells of all but a few atomic
    constituents can be considered as:
         (1) tightly bound (material is an insulator).
         (2) conduction electrons (material is a conductor).

    The material is assumed to be an insulator.
    Do you want to switch to the other (Y/N)? N

```

```

                        Calculating main results...

```

EPSTAR 5

```
┌─────────────────────────────────────────────────────────────────────┐
│                          Electrons in Methane                        │
│                                                                       │
│              Composition (Constituent Z : Fraction by weight)         │
│                                                                       │
│                      1: 0.251306 6: 0.748694                          │
│                                                                       │
│   <Z/A> = 0.623340        I = 41.7 eV      DENSITY = 6.679E-04 g/cm3   │
│                                                                       │
│   ENERGY          STOPPING POWER           CSDA    RADIATION  DENSITY  │
│             COLLISION  RADIATIVE   TOTAL    RANGE     YIELD    EFFECT   │
│                                                                DELTA   │
│                                                                       │
│    MeV      MeV cm2/g  MeV cm2/g  MeV cm2/g  g/cm2                     │
│                                                                       │
│   0.10000   4.995E+00  2.848E-03  4.998E+00  1.171E-02  3.199E-04  0.000E+00 │
│   1.00000   2.229E+00  9.149E-03  2.239E+00  3.640E-01  2.101E-03  0.000E+00 │
│  10.00000   2.610E+00  1.358E-01  2.745E+00  3.978E+00  2.389E-02  0.000E+00 │
│                                                                       │
│     Continue (C), Repeat (R), or Quit (Q) screen output (C/R/Q)? C     │
└─────────────────────────────────────────────────────────────────────┘
```

```
┌─────────────────────────────────────────────────────────────────────┐
│                                                        X to Exit       │
│                                                                       │
│   Write table to a file(Y/N)? N                                       │
│                                                                       │
│   Do another calculation (Y/N)? Y                                     │
└─────────────────────────────────────────────────────────────────────┘
```

EXAMPLE 2

```
┌─────────────────────────────────────────────────────────────────────┐
│                                                        X to Exit       │
│                                                                       │
│   Kinetic energy list options:                                        │
│                                                                       │
│       1. Take default energy list (extends from 1 keV to 10 GeV).     │
│       2. Input own energy list.                                       │
│                                                                       │
│   Selection (1/2)? 1                                                  │
└─────────────────────────────────────────────────────────────────────┘
```

Selection of item 1 requires designation of an energy range.

```
┌─────────────────────────────────────────────────────────────────────┐
│                                                                       │
│   Enter minimum energy MeV to be tabulated: .15                       │
│                                                                       │
│   Enter maximum energy (MeV) to be tabulated: 5.                      │
└─────────────────────────────────────────────────────────────────────┘
```

EPSTAR 6

```
                                                    X to Exit

    Select electrons or positrons (-/+): +

    Enter name of material: Pyrex Glass
    (used in table heading)

    Enter density (g/cm3) of material: 2.23

    Abundances for constituents of the material can be input as:

        1. Relative parts by weight.
        2. Relative parts by number (partial pressures for gases).

    Selection (1/2)? 1
```

Override I-values can be included for individual constituents (? for help).

```
                                                    X to Exit

    A blank entry ends the list.
    An override I-value can be included
    for each constituent (? for help).

    Enter chemical formula for constituent # 1: SiO2

    Enter relative abundance for constituent # 1: 0.807

    Enter chemical formula for constituent # 2: B2O3

    Enter relative abundance for constituent # 2: 0.129

    Enter chemical formula for constituent # 3: Na2O

    Enter relative abundance for constituent # 3: 0.038

    Enter chemical formula for constituent # 4: Al2O3

    Enter relative abundance for constituent # 4: 0.022

    Enter chemical formula for constituent # 5:
```

A blank entry ended the list.

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The summary shows the defined material and modifications are accepted.

```
                                                          X to Exit

  Input Summary:

     #    Abundance  Formula
     1    0.80700    SiO2
     2    0.12900    B2O3
     3    0.03800    Na2O
     4    0.02200    Al2O3
  Total 0.99600

  Add constituents (Y/N)? Y
```

```
                                                          X to Exit


  A blank entry ends the list.
  An override I-value can be included
  for each constituent (? for help).

  Enter chemical formula for constituent # 5: K2O

  Enter relative abundance for constituent # 5: 0.004

  Enter chemical formula for constituent # 6:
```

The new summary reflects the changes just entered.

```
                                                          X to Exit

  Input Summary:

     #    Abundance  Formula
     1    0.80700    SiO2
     2    0.12900    B2O3
     3    0.03800    Na2O
     4    0.02200    Al2O3
     5    0.00400    K2O
  Total  1.00000

  Add constituents (Y/N)? N
```

EPSTAR 8

```
                                                              X to Exit

Based on your input, the mean excitation energy (I-value) for the material
has been calculated to be 135.4 eV. You can:
      1. Accept this value.
      2. Enter another value.
      3. Consult a list of experimentally-derived values for some materials.
Selection (1/2/3)? 2
```

Here the user decided to change the I-value.

```
                                                              X to Exit

Enter mean excitation energy (eV) for material: 134.0

In the calculation of the density-effect correction to the collision stopping
power, the atomic electrons in the outermost shells of all but a few atomic
constituents can be considered as:
      (1)  tightly bound (material is an insulator).
      (2)  conduction electrons (material is a conductor).

The material is assumed to be an insulator.
      Do you want to switch to the other (Y/N)? N
```

```
                          Calculating main results...
```

Electrons in Pyrex Glass

Composition (Constituent Z : Fraction by weight)

5: 0.040061   8: 0.539564   11: 0.028191   13: 0.011644
14: 0.377220   19: 0.003321

Z/A> = 0.497070   I = 134.0 eV   DENSITY = 2.230E+00 g/cm3

ENERGY	STOPPING POWER			CSDA RANGE	RADIATION YIELD	DENSITY EFFECT DELTA
	COLLISION	RADIATIVE	TOTAL			
MeV	MeV cm2/g	MeV cm2/g	MeV cm2/g	g/cm2		
0.15000	2.753E+00	5.086E-03	2.758E+00	3.273E-02	9.655E-04	0.000E+00
0.17500	2.527E+00	5.337E-03	2.533E+00	4.221E-02	1.110E-03	0.000E+00
0.20000	2.358E+00	5.587E-03	2.363E+00	5.244E-02	1.251E-03	0.000E+00
0.25000	2.123E+00	6.099E-03	2.129E+00	7.481E-02	1.524E-03	0.000E+00
0.30000	1.969E+00	6.631E-03	1.976E+00	9.924E-02	1.788E-03	0.000E+00
0.35000	1.862E+00	7.185E-03	1.870E+00	1.253E-01	2.047E-03	0.000E+00
0.40000	1.784E+00	7.762E-03	1.792E+00	1.526E-01	2.302E-03	9.054E-03
0.45000	1.725E+00	8.362E-03	1.734E+00	1.810E-01	2.555E-03	2.674E-02

Continue (C), Repeat (R), or Quit (Q) screen output (C/R/Q)? **C**

Electrons in Pyrex Glass

Composition (Constituent Z : Fraction by weight)

5: 0.040061   8: 0.539564   11: 0.028191   13: 0.011644
14: 0.377220   19: 0.003321

<Z/A> = 0.497070   I = 134.0 eV   DENSITY = 2.230E+00 g/cm3

ENERGY	STOPPING POWER			CSDA RANGE	RADIATION YIELD	DENSITY EFFECT DELTA
	COLLISION	RADIATIVE	TOTAL			
MeV	MeV cm2/g	MeV cm2/g	MeV cm2/g	g/cm2		
0.50000	1.680E+00	8.983E-03	1.689E+00	2.103E-01	2.806E-03	4.648E-02
0.55000	1.644E+00	9.624E-03	1.654E+00	2.402E-01	3.057E-03	6.773E-02
0.60000	1.616E+00	1.029E-02	1.627E+00	2.707E-01	3.309E-03	9.011E-02
0.70000	1.575E+00	1.166E-02	1.587E+00	3.330E-01	3.812E-03	1.372E-01
0.80000	1.548E+00	1.311E-02	1.561E+00	3.965E-01	4.320E-03	1.862E-01
0.90000	1.530E+00	1.462E-02	1.544E+00	4.610E-01	4.832E-03	2.361E-01
1.00000	1.517E+00	1.619E-02	1.533E+00	5.260E-01	5.350E-03	2.861E-01
1.25000	1.502E+00	2.033E-02	1.522E+00	6.898E-01	6.670E-03	4.093E-01

Continue (C), Repeat (R), or Quit (Q) screen output (C/R/Q)? **C**

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```
                    Electrons in Pyrex Glass

            Composition (Constituent Z : Fraction by weight)

      5: 0.040061      8: 0.539564      11: 0.028191      13: 0.011644
     14: 0.377220    19: 0.003321

   <Z/A>  = 0.497070     I = 134.0 eV      DENSITY = 2.230E+00 g/cm3

   ENERGY          STOPPING POWER              CSDA     RADIATION  DENSITY
             COLLISION  RADIATIVE    TOTAL      RANGE      YIELD    EFFECT
                                                                    DELTA
    MeV      MeV cm2/g  MeV cm2/g  MeV cm2/g    g/cm2

   1.50000   1.498E+00  2.475E-02  1.523E+00   8.541E-01  8.025E-03 5.274E-01
   1.75000   1.500E+00  2.940E-02  1.529E+00   1.018E+00  9.411E-03 6.393E-01
   2.00000   1.504E+00  3.425E-02  1.539E+00   1.181E+00  1.083E-02 7.451E-01
   2.50000   1.517E+00  4.447E-02  1.562E+00   1.504E+00  1.373E-02 9.395E-01
   3.00000   1.531E+00  5.527E-02  1.587E+00   1.821E+00  1.672E-02 1.114E+00
   3.50000   1.545E+00  6.655E-02  1.611E+00   2.134E+00  1.977E-02 1.274E+00
   4.00000   1.558E+00  7.821E-02  1.636E+00   2.442E+00  2.286E-02 1.419E+00
   4.50000   1.570E+00  9.017E-02  1.660E+00   2.745E+00  2.600E-02 1.554E+00
   5.00000   1.580E+00  1.024E-01  1.683E+00   3.044E+00  2.916E-02 1.680E+00

        Continue (C), Repeat (R), or Quit (Q) screen output (C/R/Q)? C
```

```
                                                          X to Exit

   Write table to a file(Y/N)? Y

   Enter filename: PYREX.POS

   Do another calculation (Y/N)? N
```

EPSTAR 11

Appendix B

EXPERIMENTALLY DERIVED I-VALUES

Experimentally-derived I-values for some materials, as given in ICRU Report 37, are given in the following tables.

A. Gas Compounds

Compound	$I_{exp}(eV)$
ammonia, NH_3	53.7
butane, C_4H_{10}	48.3
carbon dioxide, CO_2	85.0
ethane, C_2H_6	45.4
heptane, C_7H_{16}	49.2
hexane, C_6H_{14}	49.1
methane, CH_4	41.7
nitric oxide, NO	87.8
nitrous oxide, N_2O	84.9
octane, C_8H_{18}	49.5
pentane, C_5H_{12}	48.2
propane, C_3H_8	47.1
water vapor, H_2O	71.6

B. Liquid Compounds

Compound	$I_{exp}(eV)$
acetone, C_3H_6O	64.2
aniline, $C_6H_5NH_2$	66.2
benzene, C_6H_6	63.4
n-butyl alcohol, C_4H_9OH	59.9
carbon tetrachloride, CCl_4	166.3
chlorobenzene, C_6H_5Cl	89.1
chloroform, $CHCl_3$	156.0
cyclohexane, C_6H_{12}	56.4
1,2-dichlorobenzene, $C_6H_4Cl_2$	106.5
dichlorodiethyl ether, $C_4Cl_2H_8$	103.3

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B. Liquid Compounds – continued

Compound	I_{exp} (eV)
1,2-dichloroethane, $C_2Cl_2H_4$	111.9
diethyl ether, $C_4H_{10}O$	60.0
ethyl alcohol, C_2H_5OH	62.9
glycerol, $C_3H_5O_3H_3$	72.6
n-heptane, C_7H_{16}	54.4
n-hexane, C_6H_{14}	54.0
methanol, CH_3OH	67.6
nitrobenzene, $C_6H_5NO_2$	75.8
n-pentane, C_5H_{12}	53.6
n-propyl alcohol, C_3H_7OH	61.1
pyridine, C_5H_5N	66.2
styrene, C_8H_8	64.0
tetrachloroethylene, C_2Cl_4	159.2
toluene, C_7H_8	62.5
trichloroethylene, C_2Cl_3H	148.1
water, H_2O	75.0
xylene, C_8H_{10}	61.8

C. Solid Compounds

Compound	I_{exp} (eV)
adenine, $C_5H_5N_5$	71.4
guanine, $C_5H_5N_5O$	75.0
nylon, type 6, $(C_6H_{11}NO)n$	63.9
paraffin wax, $C_{25}H_{25}$	48.3
polyethylene, $(C_2H_4)n$	57.4
polymethyl methacrylate, $(C_5H_8O_2)n$	74.0
polystyrene, $(C_8H_8)n$	68.7
aluminum oxide, Al_2O_3	145.2
calcium fluoride, CaF_2	166.
lithium fluoride, LiF	94.
polytetrafluoroethylene, "Teflon", $(C_2F_4)n$	99.1
silicon dioxide, SiO_2	139.2
A-150 tissue-equivalent plastic	65.1
standard nuclear-research photographic emulsion	331.

Appendix C

HELP SCREENS

The following pages are actual Help Screens which the user encounters when running the Electron and Positron Stopping Powers and Ranges Program. The individual screens are available for each function (command) while running the program by entering a question mark.

General Background

SCREEN CONTROL: If your last screen displayed the characters "[2J" at the upper left, you need to:
1. Add the line "DEVICE = ANSI.SYS" to your CONFIG.SYS file
2. Make sure the file ANSI.SYS is in your root directory
3. Re-boot the computer, and begin again

QUANTITIES CALCULATED: This code calculates stopping powers, ranges, and related quantities in the material you specify, for electrons or positrons with kinetic energies you specify (in the range from 1 keV to 10 GeV). The results include:

COLLISION STOPPING POWER - the average energy loss per unit pathlength due to inelastic Coulomb collisions with bound atomic electrons of the medium resulting in ionization and excitation. Units are Mev cm2/g.

RADIATIVE STOPPING POWER - the average energy loss per unit pathlength due to the emission of bremsstrahlung in the field of the atomic nucleus and of the atomic electrons. Units are Mev cm2/g.

TOTAL STOPPING POWER - the sum of the collision and radiative stopping powers.

CSDA RANGE - the pathlength traveled in slowing down to rest (assuming that the energy loss per unit pathlength at any point along the path is given by the total stopping power). Units are g/cm2.

RADIATION YIELD - the fraction of kinetic energy converted to bremsstrahlung in slowing down to rest (calculated in the continuous-slowing-down-approximation, CSDA). Quantity is dimensionless.

EPSTAR 14

DENSITY EFFECT DELTA - the density-effect correction incorporated into the Bethe formula, which accounts for the reduction of the collision stopping power due to the polarization of the medium. Quantity is dimensionless.

It is recommended that the user be somewhat familiar with stopping-power theory. This code will give results consistent with those found in NBSIR82-2550-A (1983), "Stopping Powers and Ranges of Electrons and Positrons (2nd Ed.)", M.J. Berger and S.M. Seltzer, National Bureau of Standards, Gaithersburg, MD 20899, and in ICRU Report 37 (1984), "Stopping Powers for Electrons and Positrons", International Commission on Radiation Units and Measurements, Bethesda, MD 20814.

Results for the radiative stopping power will be slightly different from those found in these references, because this version of this program incorporates updated radiative energy-loss data given by S.M. Seltzer and M.J. Berger, Atomic Data and Nuclear Data Tables, 35, 345 (1986).

Results for the collision stopping power are calculated according to Bethe's formula, and depend on the values for (1) the density of the material, and (2) the mean excitation energy (or I-value) of the material. The density enters only indirectly, through the density-effect correction. This correction also depends on the I-value and on how the outermost-shell atomic electrons are treated (either as tightly bound or conduction electrons). The I-value enters directly, but logarithmically. The rules this program uses to predict the I-value generally depend on (a) whether the material is in the gas or condensed phase, and (b) whether atomic constituents of the material are present in their elemental (or pure molecular) form or in a compound.

This program assumes materials with densities less than 0.1 g/cm3 to be in the gas phase, and those with greater densities to be in the condensed phase. There is presently no mechanism in the code to override this choice.

As the default, this program assumes that materials with more than a single atomic constituent are compounds.This should be overridden for those constituents that are present in their elemental form, that is, in a mixture rather than in a compound. A good example is air, in which N2, O2 and Ar should be assigned their elemental values. The override can be done when specifying the composition of the material, by appending a single character to the chemical formula for that constituent.

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A similar override can also be used for any constituent compound or element, to specify an I-value different from that predicted by this program (say, one that is experimentally known). FURTHER DETAILS ARE AVAILABLE IN A HELP SCREEN OBTAINED BY ENTERING A "?" AT THE PROMPT FOR CONSTITUENT CHEMICAL FORMULAS.

There is also an option to enter the I-value for the material as a whole, which takes precedence over any previous assignments.

FUTURE HELP: At most of the prompts you can enter a "?" to get further explanation.

***** End of Help *****

Energy List

OPTION 1. The default list consists of 113 kinetic energies and covers the range from 1 keV to 10 GeV, using a moderately-fine quasi-logarithmic grid. If this option is chosen, you will be asked for values (in MeV) of the minimum and maximum kinetic energies you want to be tabulated, enabling you to select only the energy range in which you are interested.

OPTION 2. If you chose to input you own list of kinetic energies, you will be prompted for each energy. To end the input of energies, simply strike ENTER at the next prompt. This program can accept up to 120 energies; if more than this are entered, the code will abort. The energies are tested as you enter them, and those outside the permissible range (from 0.001 to 10000 MeV) are rejected. Regardless of the order entered, the energies will be sorted into a list of monotonically increasing values.

You should be aware that the Bethe formula, used to calculate the collision stopping power, becomes less reliable at low energies. For materials of high atomic number, the accuracy of the results are known to deteriorate quickly below, say, 10 keV; for low-Z materials, the results should be reasonably good down to 1 keV. A conservative estimate of the accuracy of the collision stopping power calculated at 1 keV has been stated to be approximately (I/7) percent, where I is the value in eV of the mean excitation energy for the material.

***** End of Help *****

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Incident Particle Designation

The calculations can be done for:
electrons (enter "-")
positrons (enter " + ")

The supplied default is "-", and allows you to simply strike ENTER to select electrons.

***** End of Help *****

Name of Target Material

This name is used only for making the table heading in the display of the calculated results. The name can be up to 68 characters long. Leading and trailing blanks are ignored; imbedded blanks are retained. The portion of the table heading into which this name is merged will be written as:

Electrons in "name"   *or*   Positrons in "name"

so, for elegance, you should choose the use of upper/lower case accordingly.

***** End of Help *****

Material Density Designation

The density is not used to calculate results in linear units (e.g., MeV/cm); all results are given in terms of mass units in which pathlength has units of g/cm2. However, the density enters indirectly into the calculation of the stopping power in two ways.

The density is used to determine whether the material is in the gas or condensed phase. This program assumes that materials with densities less than 0.1 g/cm3 are gases, and those with densities greater than 0.1 g/cm3 are liquids or solids. The assumed state of aggregation affects the prediction of the value for the mean excitation of the material, which is the key parameter in the Bethe formula for the collision stopping power.

The density is also used in the calculation of the density-effect correction incorporated into the Bethe formula, which accounts for the reduction of the collision stopping power due to the polarization of the medium.

If the material is a gas, you can enter its density for any convenient conditions of temperature and pressure. This program will ask you the temperature and pressure for which the density was specified, and ask you the temperature and pressure for which you want the calculation done. The density will be adjusted according to the Boyle and Charles-Gay-Lussac laws.

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If a density value of 0 (zero) in entered, this program will treat (with your concurrence) the material as an ideal gas and calculate the density accordingly.

<div align="center">***** End of Help *****</div>

Ideal Gas Calculation

If you want the program to treat the material as an ideal gas, the density will be assumed given by M/V, where M is the gram molecular weight of the gas and V is the mol volume of 22414 cm3 at standard conditions (0 deg C and 1 atm).

Subsequent prompts ask you for the temperature and pressure desired for the calculation, and the density will be adjusted accordingly.

<div align="center">***** End of Help *****</div>

Gas Parameters

The density you entered indicates that the material is a gas. Here the program asks you the temperature and pressure for which the density was specified, and will subsequently ask you the temperature and pressure for which you want the calculation done. The density will be adjusted according to the Boyle and Charles-Gay-Lussac laws.

<div align="center">***** End of Help *****</div>

Target Material Composition

The composition of the material is specified by entering information on each of its constituents. Any of these constituents can be either single elements or molecular compounds. The final material is determined by adding the constituents in proportion to the relative abundances that are entered.

OPTION 1. The relative abundance of each constituent is entered in terms of parts by weight.

OPTION 2. The relative abundance of each constituent is entered in terms of parts by number (partial pressures for gases). A zero or negative value is permissable, but you will be asked if you want to reenter it.

Option 2 can be handy for gas mixtures that are specified in terms of partial pressures or - equivalently - parts by volume. In this case it will be important to specify correctly the complete molecular formula for the constituents (e.g., N2 and O2, rather than N and O, in air).

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Option 2 can also be used to build molecules, or to build a material from numbers of compounds. For example, 6 C's + 10 H's + 5 O's would give C6H10O5, although it would be simpler to enter the complete formula as a single constituent. The following scheme is also possible: 1 (C6H10O5) - 2.3 (OH) + 2.3 (ONO2) would give the composition of nitrated cellulose.

If there is only a single constituent (either an element or a molecular compound), it is irrelevant which option is chosen.

You may use any normalization for the relative abundances that you find convenient. After all constituents are entered, EPSTAR displays a summary table including the total relative abundance. The total will be renormalized to unity for the final calculations.

***** End of Help *****

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Constituent Designation and I-Values

The material is specified by entering information on each of its constituents. Any of these constituents can be either single elements or molecules. This program can accept up to 30 constituent chemical formulas. The final material will be determined by adding these constituents in proportion to the relative abundances that will also be entered. The total number of different atomic species in the final material cannot exceed 30.

When there are no further constituents, simply strike ENTER at the prompt.

CHEMICAL FORMULAS. The chemical formula for each constituent is entered as you would type it, as any combination of the standard chemical symbols for the elements followed by their number of atoms in the molecule. The length of each formula (including any I-value override, explained below) is restricted to 72 characters. Each chemical formula can include up to 30 elemental chemical symbols. The chemical symbols must be entered with the proper use of upper and lower case; the number of atoms must be whole numbers (integers) and can be no larger than 999,999. If the number of atoms is not given, it is assumed to be one. No parentheses are allowed, such as in Ce2(SO4)3 or in (C2H4)n. The symbols for the elements in the molecule can appear in any order, and can be repeated in the formula. Blanks are ignored.

Examples: Si
           H2O
           HOH
           Ce2S3O12
           C2H5OH

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This program will indicate any failure to understand your input, and prompt you to re-enter the formula.

MEAN EXCITATION ENERGIES. The default value of the mean excitation energy (or I-value) for each constituent is predicted by this program using a modified Bragg additivity algorithm, which - at least approximately - takes into account chemical binding effects (pure element or compound) and phase effects (gas or condensed). You may wish to override the default value for a constituent for one of the following two reasons.

(1) If only a single chemical symbol is entered to specify the whole material, then this program assumes that the final material is a pure element. Otherwise, it is assumed that the elements entered are all present in chemical compounds, and their compound I-values are to be used (except for the rare gases). Thus, for a real mixture containing constituents that are present in their elemental state, the I-value for the material would be somewhat in error. To force the use of elemental I-values for a constituent defined by a single appearance of a single chemical symbol, simply append the character "@" (the "at" symbol, above the 2 on the keyboard) after the chemical symbol. For example, for the oxygen in air you should enter O2@, and for the nitrogen N2@. Other constituents entered at their own prompt would be unaffected unless they were also marked with a "@". When constituents are defined by more than a single appearance of a single chemical symbol, only these marked with a "@" will be affected (however, see (2) below). If only a single elemental constituent is to be entered (i.e., you are specifying a pure element), it is not necessary to use the "@".

(2) A different, or better, I-value may be available for the constituent than is predicted in this program. This applies to any constituent, whether comprised of single or multiple atomic species. In this case, after the chemical formula, append the character "@" followed by the I-value (in eV) you wish to use. For example, entering H2O@75.0 would specify water with a mean excitation energy of 75.0 eV. (The I-value can be entered as a whole number, without the decimal point.) If the I-value is omitted and the constituent is defined by a chemical formula consisting of only a single chemical symbol, then you force the elemental I-value; if the constituent formula has multiple chemical symbols, there is no effect.

Experimentally-derived I-values for compounds, as given in ICRU Report 37, are given in the following tables.

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A. Gas Compounds

Compound	$I_{exp} (eV)$
ammonia, NH_3	53.7
butane, C_4H_{10}	48.3
carbon dioxide, CO_2	85.0
ethane, C_2H_6	45.4
heptane, C_7H_{16}	49.2
hexane, C_6H_{14}	49.1
methane, CH_4	41.7
nitric oxide, NO	87.8
nitrous oxide, N_2O	84.9
octane, C_8H_{18}	49.5
pentane, C_5H_{12}	48.2
propane, C_3H_8	47.1
water vapor, H_2O	71.6

B. Liquid Compounds

Compound	$I_{exp} (eV)$
acetone, C_3H_6O	64.2
aniline, $C_6H_5NH_2$	66.2
benzene, C_6H_6	63.4
n-butyl alcohol, C_4H_9OH	59.9
carbon tetrachloride, CCl_4	166.3
chlorobenzene, C_6H_5Cl	89.1
chloroform, $CHCl_3$	156.0
cyclohexane, C_6H_{12}	56.4
1,2-dichlorobenzene, $C_6H_4Cl_2$	106.5
dichlorodiethyl ether, $C_4Cl_2H_8$	103.3
1,2-dichloroethane, $C_2Cl_2H_4$	111.9
diethyl ether, $C_4H_{10}O$	60.0
ethyl alcohol, C_2H_5OH	62.9
glycerol, $C_3H_5O_3H_3$	72.6
n-heptane, C_7H_{16}	54.4
n-hexane, C_6H_{14}	54.0
methanol, CH_3OH	67.6
nitrobenzene, $C_6H_5NO_2$	75.8
n-pentane, C_5H_{12}	53.6
n-propyl alcohol, C_3H_7OH	61.1
pyridine, C_5H_5N	66.2
styrene, C_8H_8	64.0
tetrachloroethylene, C_2Cl_4	159.2
toluene, C_7H_8	62.5
trichloroethylene, C_2Cl_3H	148.1
water, H_2O	75.0
xylene, C_8H_{10}	61.8

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C. Solid Compounds

Compound	$I_{exp}(eV)$
adenine, $C_5H_5N_5$	71.4
guanine, $C_5H_5N_5O$	75.0
nylon, type 6, $(C_6H_{11}NO)n$	63.9
paraffin wax, $C_{25}H_{25}$	48.3
polyethylene, $(C_2H_4)n$	57.4
polymethyl methacrylate, $(C_5H_8O_2)n$	74.0
polystyrene, $(C_8H_8)n$	68.7
aluminum oxide, Al_2O_3	145.2
calcium fluoride, CaF_2	166.
lithium fluoride, LiF	94.
polytetrafluoroethylene, "Teflon", $(C_2F_4)n$	99.1
silicon dioxide, SiO_2	139.2
A-150 tissue-equivalent plastic	65.1
standard nuclear-research photographic emulsion	331.

***** End of Help *****

Negative Abundances

If you choose, the zero or negative value will be accepted, and will have the obvious effect in your specification of the material. If the TOTAL of all abundances entered is not greater than zero, you will be asked to begin again the entering of the constituents.

***** End of Help *****

Calculated I-values

Results for the collision stopping power are calculated according to Bethe's formula, and depend logarithmically on the value for the mean excitation energy (or I-value) of the material. The default I-value predicted by this program for the material as a whole is based on a modified Bragg additivity algorithm, which - at least approximately - takes into account chemical binding effects (pure element or compound) and phase effects (gas or condensed). This value may not be the most accurate one; you may substitute a value of your choice.

Experimentally-derived I-values for some materials, as given in ICRU Report 37, are given in the following tables.

EPSTAR 22

A. Gas Compounds

Compound	$I_{exp}(eV)$
ammonia, NH_3	53.7
butane, C_4H_{10}	48.3
carbon dioxide, CO_2	85.0
ethane, C_2H_6	45.4
heptane, C_7H_{16}	49.2
hexane, C_6H_{14}	49.1
methane, CH_4	41.7
nitric oxide, NO	87.8
nitrous oxide, N_2O	84.9
octane, C_8H_{18}	49.5
pentane, C_5H_{12}	48.2
propane, C_3H_8	47.1
water vapor, H_2O	71.6

B. Liquid Compounds

Compound	$I_{exp}(eV)$
acetone, C_3H_6O	64.2
aniline, $C_6H_5NH_2$	66.2
benzene, C_6H_6	63.4
n-butyl alcohol, C_4H_9OH	59.9
carbon tetrachloride, CCl_4	166.3
chlorobenzene, C_6H_5Cl	89.1
chloroform, $CHCl_3$	156.0
cyclohexane, C_6H_{12}	56.4
1,2-dichlorobenzene, $C_6H_4Cl_2$	106.5
dichlorodiethyl ether, $C_4Cl_2H_8$	103.3
1,2-dichloroethane, $C_2Cl_2H_4$	111.9
diethyl ether, $C_4H_{10}O$	60.0
ethyl alcohol, C_2H_5OH	62.9
glycerol, $C_3H_5O_3H_3$	72.6
n-heptane, C_7H_{16}	54.4
n-hexane, C_6H_{14}	54.0
methanol, CH_3OH	67.6
nitrobenzene, $C_6H_5NO_2$	75.8
n-pentane, C_5H_{12}	53.6
n-propyl alcohol, C_3H_7OH	61.1
pyridine, C_5H_5N	66.2
styrene, C_8H_8	64.0
tetrachloroethylene, C_2Cl_4	159.2
toluene, C_7H_8	62.5
trichloroethylene, C_2Cl_3H	148.1
water, H_2O	75.0
xylene, C_8H_{10}	61.8

EPSTAR 23

C. Solid Compounds

Compound	$I_{exp}(eV)$
adenine, $C_5H_5N_5$	71.4
guanine, $C_5H_5N_5O$	75.0
nylon, type 6, $(C_6H_{11}NO)n$	63.9
paraffin wax, $C_{25}H_{25}$	48.3
polyethylene, $(C_2H_4)n$	57.4
polymethyl methacrylate, $(C_5H_8O_2)n$	74.0
polystyrene, $(C_8H_8)n$	68.7
aluminum oxide, Al_2O_3	145.2
calcium fluoride, CaF_2	166.
lithium fluoride, LiF	94.
polytetrafluoroethylene, "Teflon", $(C_2F_4)n$	99.1
silicon dioxide, SiO_2	139.2
A-150 tissue-equivalent plastic	65.1
standard nuclear-research photographic emulsion	331.

***** End of Help *****

Density Effect Correction

The density-effect correction is incorporated into the Bethe formula for the collision stopping power in order to take into account the reduction in the stopping power due to the polarization of the medium. The calculation of the density-effect correction is done using a rather simple, but effective, model in which the material can be treated either:

(1) as an insulator (electrons in the outermost shells of all constituent atoms are considered tightly bound); or,

(2) as a conductor (electrons in the outermost shells of most constituent atoms are considered to be conduction electrons).

This program has a built-in table for the number of outer-shell electrons that can be assigned as conduction electrons for each element in the periodic chart (these data are given in the file BINDENGY.DAT). For a few elements, no electrons can be assigned to be conduction electrons, regardless of the choice you make; these presently include He, O, F, Ne, Ar, Kr, Xe, At, and Ra. Thus, the option presented to you offers the choice of (1) treating no electrons as conduction electrons, or (2) treating all of those pre-assigned by this program as conduction electrons.

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The effect of this choice on the final values of the collision stopping power is usually less than about 0.5%, but has been found to be as large as about 2%. These are maximum differences which occur in the most sensitive energy range; they are smaller at other energies. The effects of using somewhat different assignments in BINDENGY.DAT have not been fully explored; however, it is expected that other reasonable assignments would lead to changes within these same limits.

This program makes an initial choice whether to treat the material as an insulator or as a conductor for the purpose of calculating the density-effect correction. This is presently done according to the following rule: if the material contains any amount of H, He, N, O, F, Ne, P, S, Cl, Ar, Br, Kr, I, Xe, At, or Rn, it is classified as an insulator. You are given the opportunity to change this default selection. In ICRU Report 37, only condensed-phase metals were treated as conductors for the purpose of calculating the density-effect correction. Perhaps a reasonable rule is that if the majority of the outer-shell atomic electrons in the material as a whole are known to be conduction electrons, then the material should be treated as a conductor.

***** End of Help *****

Repeat Designated Material

This option allows you to continue to do calculations for the material you last defined (with no changes in any of the material specifications).

This may be useful when you want to change only the energy list, or to switch between electrons and positrons.

***** End of Help *****

Appendix D

CONTACTS

If you have questions or comments about the database, the Standard Reference Data Program would like to hear from you. Also, if you have any problems with the diskettes or installation, please let us know by contacting:

> Joan Sauerwein
> National Institute of Standards and Technology
> Standard Reference Data
> Building 820, Room 113
> Gaithersburg, MD 20899
> Internet: srdata@nist.gov
> Phone: (301) 975-2208
> FAX: (301) 926-0416

If you have technical questions relating to the data, contact:

> Jean W. Gallagher
> National Institute of Standards and Technology
> Standard Reference Data
> Building 820, Room 113
> Gaithersburg, MD 20899
> Phone: (301) 975-2204

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