

NIST Standard Reference Database 71

NIST Electron Inelastic-Mean-Free-Path Database

Version 1.2

Users' Guide

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I. INTRODUCTION

This database provides values of electron inelastic mean free paths (IMFPs) in solid elements and compounds at selected electron energies between 50 eV and 10,000 eV (although most of the available data are for energies less than 2,000 eV).

The database was designed mainly to provide IMFPs for applications in surface analysis by Auger-electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). For these applications, IMFPs are needed for quantitative surface analyses (to correct elemental sensitivity factors for variations of IMFP with chemical state), for defining the surface sensitivity, and in calculations of the transport of signal electrons in solids. The IMFPs are also useful for defining the surface sensitivity of other surface-characterization methods in which electron beams are employed and for applications in which knowledge of the transport of low-energy electrons in solids is needed.

In AES and XPS, a user often needs IMFP values at one or more specified electron energies or wishes to display IMFPs as a function of energy. The database can provide IMFP information from up to three types of sources: calculated IMFPs from experimental optical data for a limited number of materials, IMFPs measured by elastic-peak electron spectroscopy (EPES) for some elemental solids, and IMFPs from predictive formulae for all materials. The calculated and measured IMFPs were generally reported in journal papers at specified electron energies, and it was convenient to fit these IMFPs with appropriate functions so that IMFPs could be found by interpolation for intermediate energies [1].

A user of this database can obtain and display IMFP values for elements, inorganic compounds, and organic compounds at specified electron energies or energy ranges. For a selected material in each class, the user can specify a source of IMFPs (calculations, measurements, or predictive formulae) and then choose from a number of options for the IMFP units (nanometers, Ångstroms, or milligrams per square meter) and the type of display (linear, logarithmic, or linear/logarithmic coordinates).

The user can display the IMFP results graphically (that is, a plot of IMFP versus electron energy), obtain an IMFP for a selected electron energy, obtain IMFPs for a number of specified energies, and create an IMFP Table for regularly spaced electron energies. The IMFPs from the latter two options can be stored in files for later processing (e.g., on-screen comparisons of IMFPs from different sources for the same material or comparisons of IMFPs for different materials), printing, or permanent storage. Finally, graphical displays can be saved in Windows bitmap format for easy incorporation into other documents.

NIST released version 1.0 of the Electron Inelastic-Mean-Free-Path Database (SRD 71) in September, 1999. Version 1.0 was designed to operate under the DOS operating system. Version 1.1 was designed to operate under the Windows 95, Windows 98, or Windows NT operating systems, and was released in December, 2000. The database screens were redesigned to make use of the database easier and more convenient. There were no changes or additions to the data in the database although there were some changes to the N_v parameter values listed in Table A.1.

The installation program for Version 1.2 was changed so that it would operate on newer versions of the Windows operating system; Version 1.2 was released in December, 2010. There were no changes or additions to the data in the database although a new About box was added to the main menu. This box shows three references, a 1999 critical review [1] and two recent reviews [2,3] that discuss evaluations of the compiled data, methods of determination, and uncertainty.

II. GETTING STARTED

Packet Content

CD-ROM

Users' Guide

Alternatively, the files on the CD-ROM and a PDF file with the Users' Guide can be downloaded from NIST (<http://www.nist.gov/srd/surface.cfm>).

System Requirements

1. Personal computer with Windows 95, Windows 98, Windows NT, Windows 2000, Windows ME, Windows XP, Windows Vista, or Windows 7 operating system
2. CD-ROM drive
3. Screen resolution: 1024 by 768 pixels.
4. System font size: small fonts.
5. Printer: Laser printer supporting the PCL 6 printer language.
6. Hard disk space: 720 kilobytes minimum. Larger amounts of storage are required if numerous files are created with the database. It is suggested that 30 Megabytes be available, particularly if graphic files are created.

The database has been designed to operate optimally at the screen resolution given above. However, it can also be operated at a lower screen resolution, e.g., 640 by 480 pixels, or 800 by 600 pixels. At higher resolutions, the database will operate correctly but there may be difficulty in reading text on the screen. For all resolutions, small system fonts must be selected.

To change the screen resolution or the system font size, follow these steps:

1. Double click the **My Computer** icon on the desktop.
2. Click the **Control panel** icon.
3. Double click the **Display** icon.
4. Click on the **Settings** tab.
5. Set a given resolution by moving the slider.

To change the system font size, proceed as follows depending on the operating system in use:

For Windows 95 or NT, select **Small Fonts** in the **Font Size** box.

For Windows 98, click on the **Advanced...** button, select the **General** tab, and then select the **Small Fonts** option in the **Display** box.

For Windows XP, click on the **Advanced...** button, and then select the **Normal size (96 DPI)** option in the **Display** box.

For Windows Vista, click on **Appearance and Personalization, Personalization, Adjust font size (DPI)** in the left pane, and select **Default scale (96 DPI)**.

For Windows 7, click on **Appearance and Personalization, Display**, and select **Small - 100 %** (default option).

Installation

1. Insert the CD-ROM into the disk drive of the computer.
2. Click the **Start** button on the task bar.
3. Click the **Run** command.
4. Type D:\SETUP (if D: is the drive letter for the disk drive) and click OK.
5. Follow instructions on the screen.

Alternatively, the following procedure can be used:

1. Insert the disk into the disk drive of the computer.
2. Double-click **My Computer** on the desktop.
3. Double-click the icon corresponding to the disk drive.
4. Double-click the **Setup** icon (showing the computer).
5. Follow instructions on the screen.

If files have been downloaded into a directory on the user's personal computer, double-click the **Setup** icon (i.e., **setup.exe**).

Should difficulty be encountered in installing the database as described above (e.g., due to security settings on the computer), the database can be launched by double-clicking on **IMFPWIN.exe** located in the Program Files directory.

By default, the database is installed in the directory C:\PROGRAM FILES\NIST\IMFPWIN. Furthermore, an IMFPWIN icon is created. This icon appears after clicking the **Start** button and choosing **Programs**.

Removal of the Database

1. Double click **My Computer** on the desktop.
2. Double click the **Control panel** icon.
3. Double click the **Add/Remove Programs** icon.
4. Select **Install/Uninstall**.
5. In the list of programs, click **Imfpwin**.
6. Click the button **Add/Remove**.

III. STRUCTURE OF THE PROGRAM

Main Menu

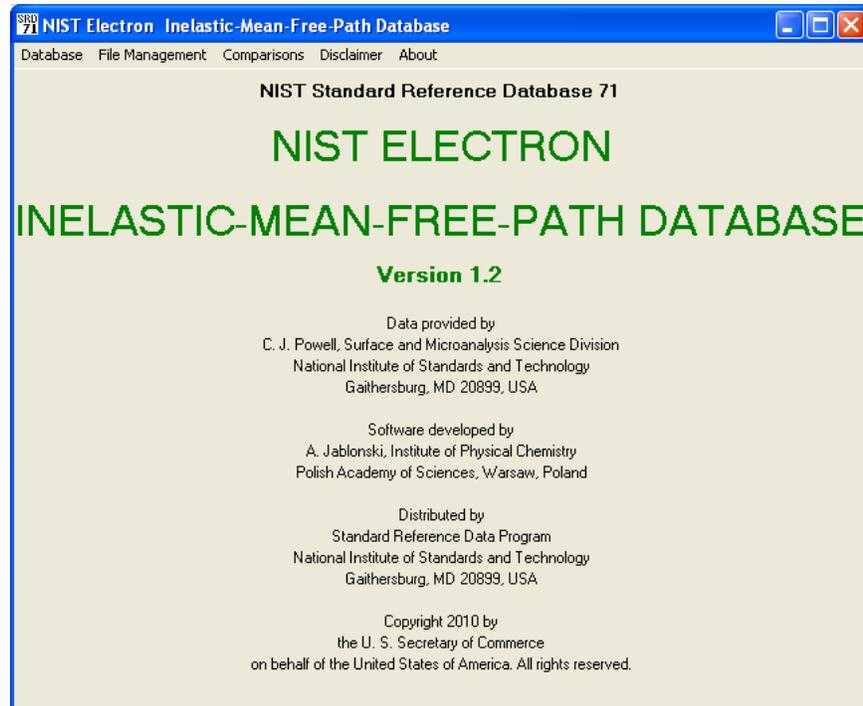


Figure 1. The title screen and main menu.

The five options of the Main Menu are listed in the upper part of the title screen (Fig. 1), and the submenus corresponding to the first three options are shown in Figs. 2, 4 and 5.

The functions of the five main menu options are as follows:

1. Database (Figure 2)

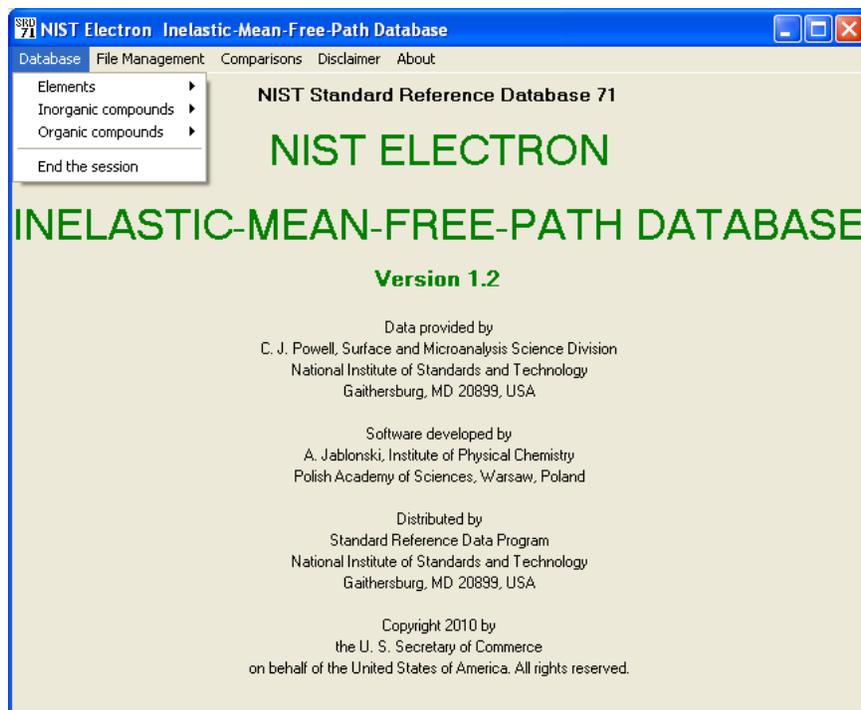


Figure 2. First option of the main menu (Database)

With this option, IMFPs can be obtained for elements, inorganic compounds, and organic compounds. For each of these three classes of materials, submenus (Figs. 3(a)-(c)) enable the selection of data sources and the types of data to be obtained. These submenus are described in Section IV. Operation of the database can be terminated by choosing End the session.

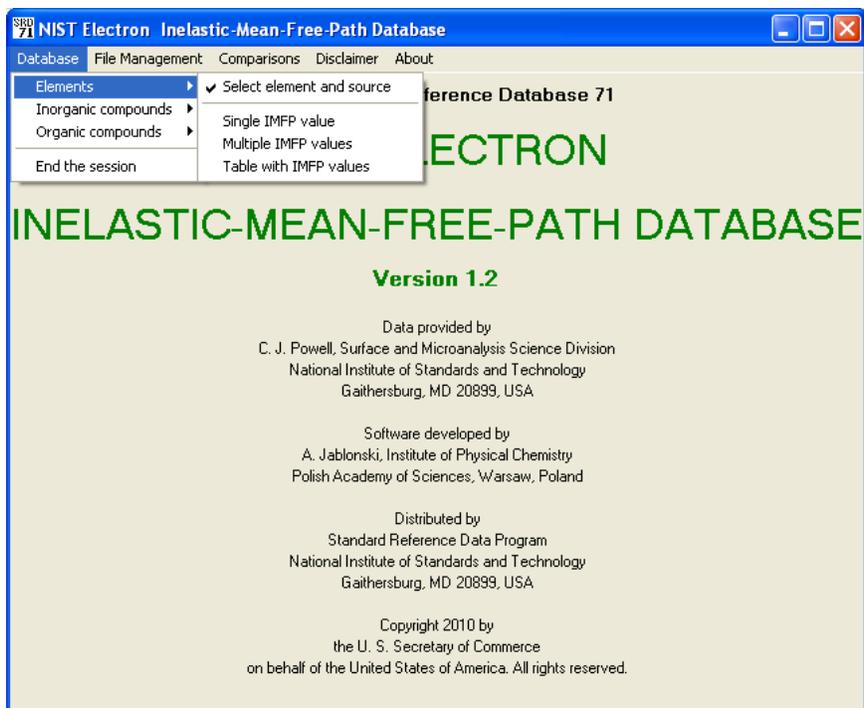


Figure 3(a). Elements submenu for the Database menu of Figure 2.

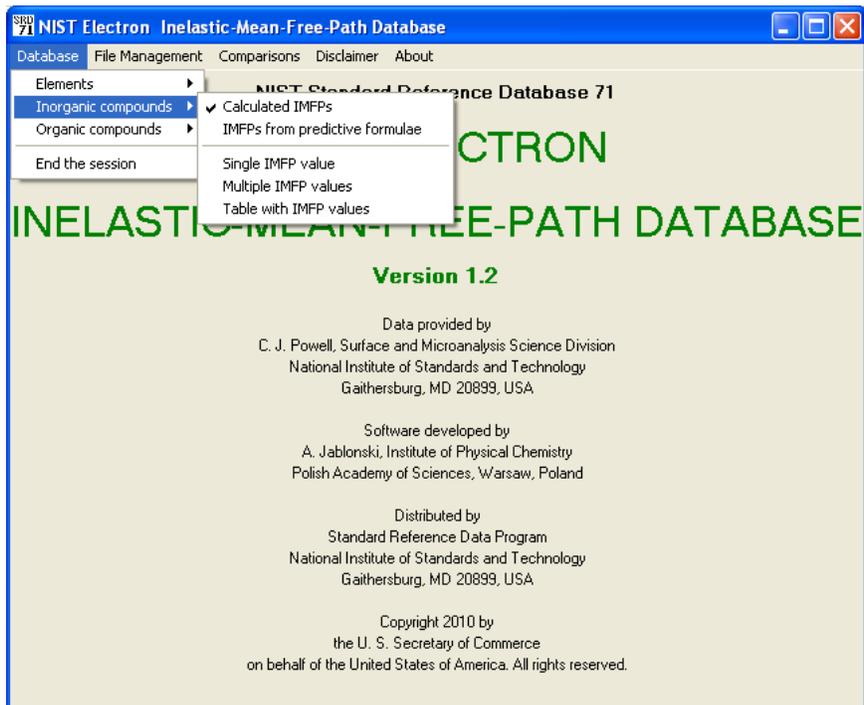


Figure 3(b). Inorganic Compounds submenu for the Database menu of Figure 2.

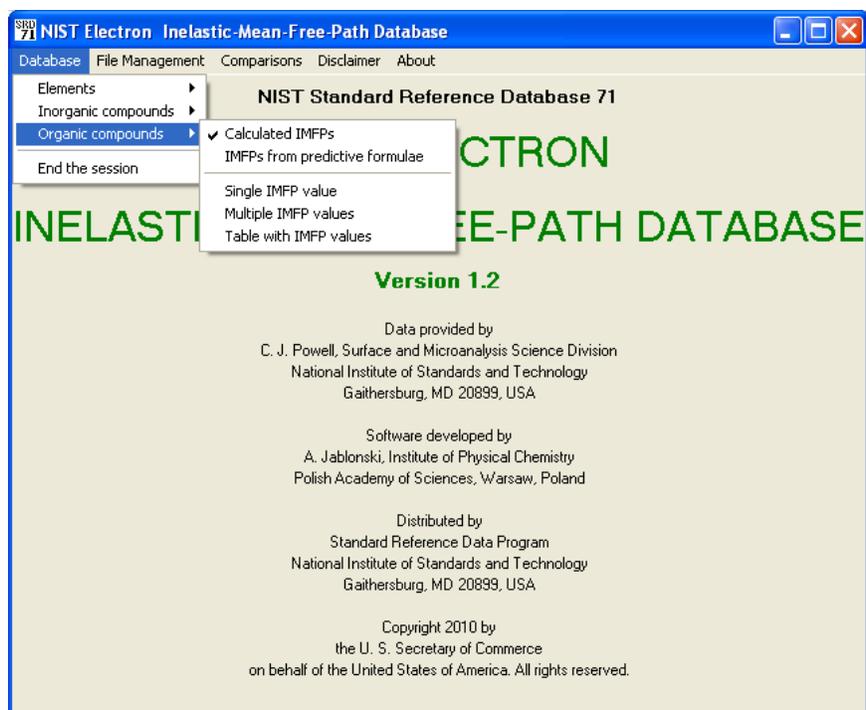


Figure 3(c). Organic compounds submenu for the Database menu of Figure 2.

2. File Management (Figure 4)

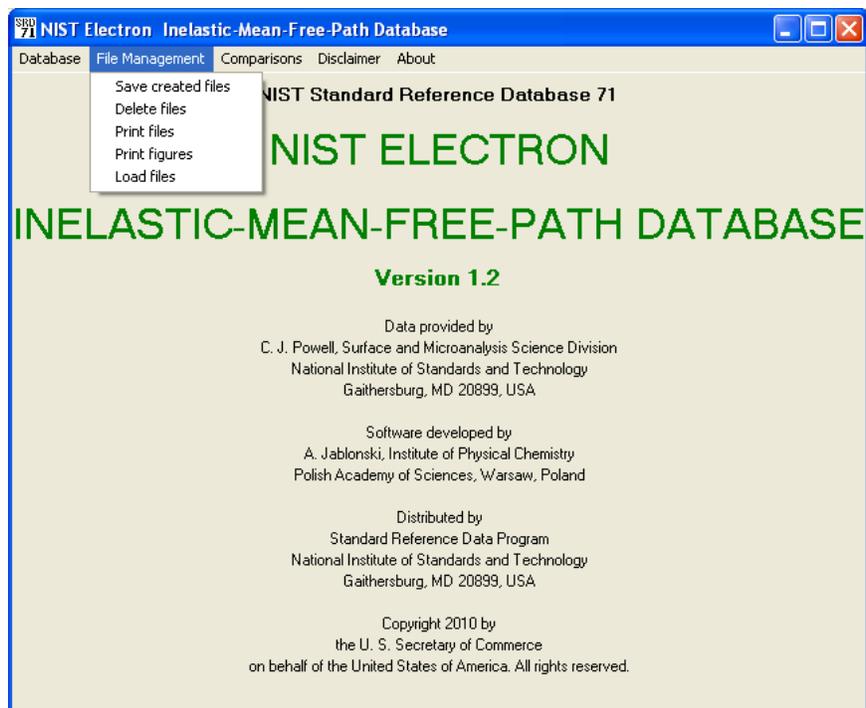


Figure 4. Second option of the main menu (File Management).

This option allows the user to save files created in the present session to another directory for permanent storage, to delete files from the database directory, to print files containing IMFP

data, to print figures showing displays of IMFP data as a function of electron energy, and to load files containing IMFP data or figures that were created in earlier sessions and stored in another directory.

3. Comparisons (Figure 5)

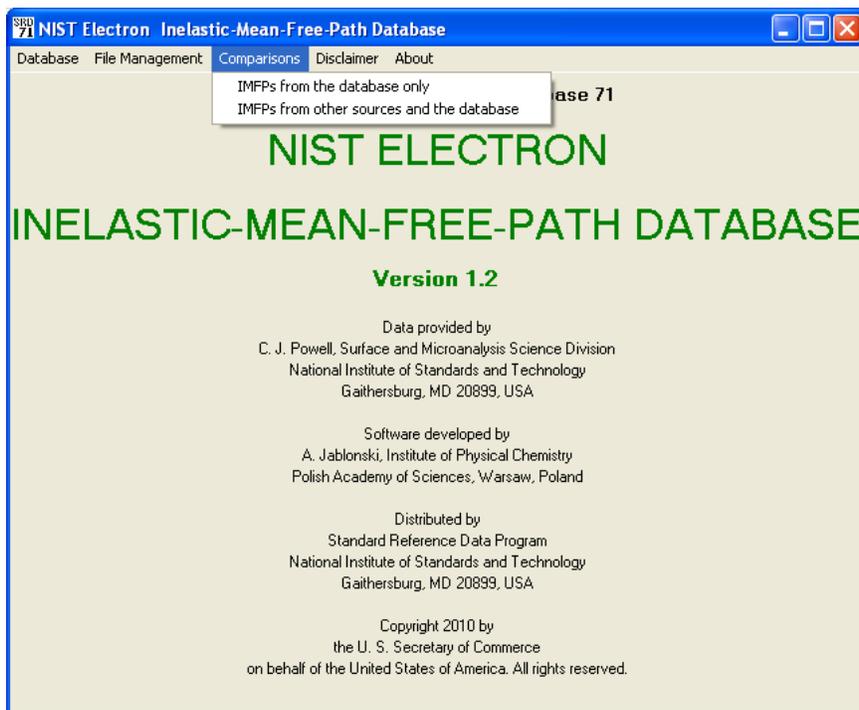


Figure 5. Third option of the main menu (Comparisons).

With this option, IMFP data for different materials and/or from different sources can be graphically compared.

4. Disclaimer (Figure 6)

The NIST disclaimer is stated.

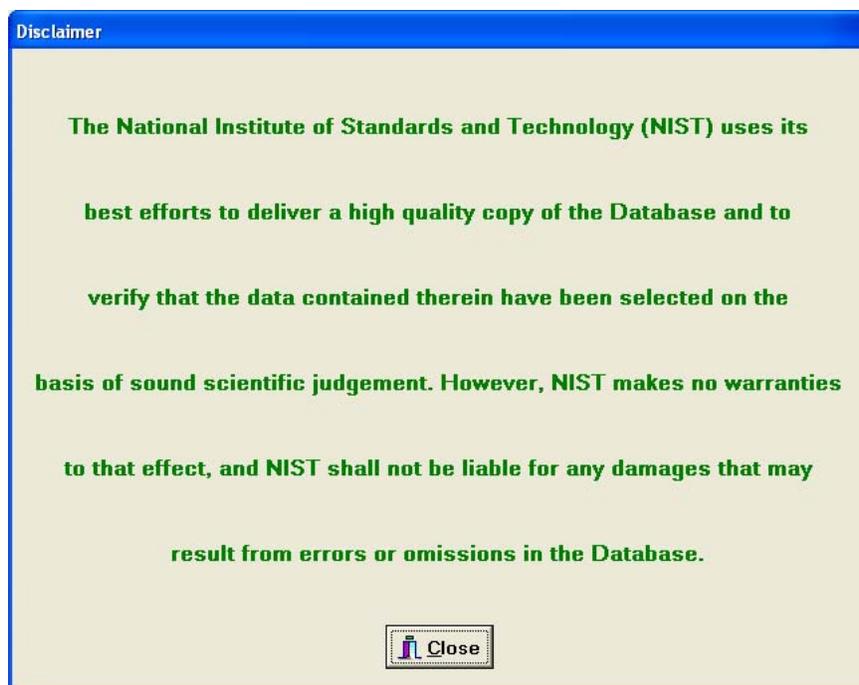


Figure 6. NIST disclaimer.

6. About box (Figure 7)

The About box gives information on the release date of this version of the database, how the database should be cited in publications, and references to evaluations of the compiled data, methods of determination, and uncertainties [1-3].

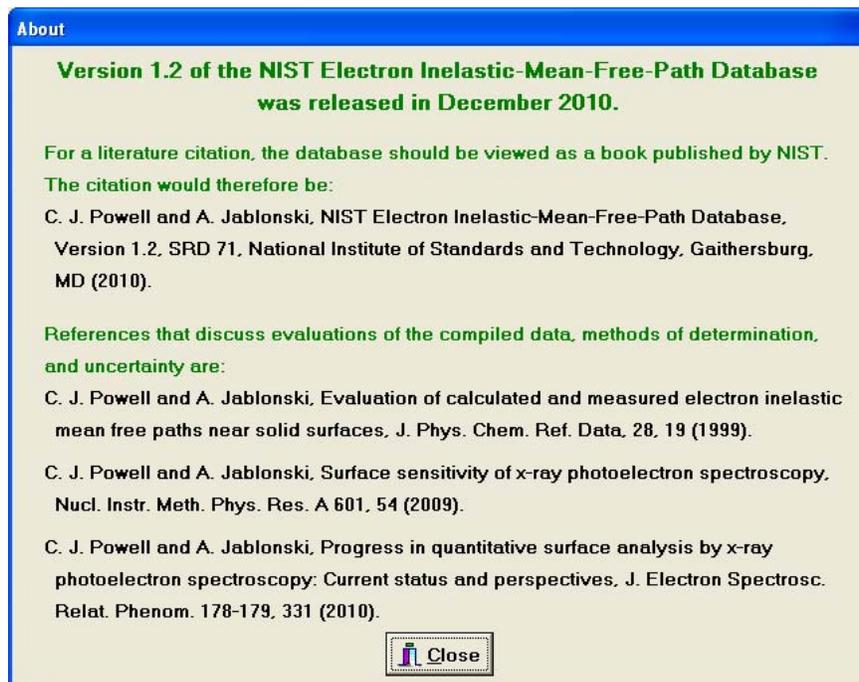


Figure 7. The About box.

V. RUNNING THE DATABASE PROGRAM

Starting the Database

The database can be started by any of the following means:

1. Click the Start button, choose Programs, and then the **IMFPWIN** icon.
2. Click the Start button, choose Run, and type:
C:\PROGRA~1\NIST\IMFPWIN\IMFPWIN,
and then click **OK**.
3. Double-click the **My Computer** icon on the desktop, select the C:\PROGRAM FILES\NIST\IMFPWIN directory, and double-click on the **IMFPWIN** icon.

Database

(First option of the main menu)

Elements

(First option of the Database option on the main menu)

The user will initially select an element and a source of data (Figure 3(a)).

The Periodic Table of the elements will then appear (Figure 8), and an element can be selected by clicking on the button for the element of interest. A selection is indicated by a change of color from black to red.

An element can be deselected by clicking again on another button. After a selection has been made (Cu in the case shown in Figure 8), the **OK** button should be clicked. Clicking on the **Cancel** button returns control to the opening screen and the main menu. Note that it is not possible to select an element shown in bold letters.

After an element has been selected, a screen will appear showing the IMFP data sources available for that element. For example, if copper (Cu) had been chosen, the screen shown in Figure 9 would be displayed.

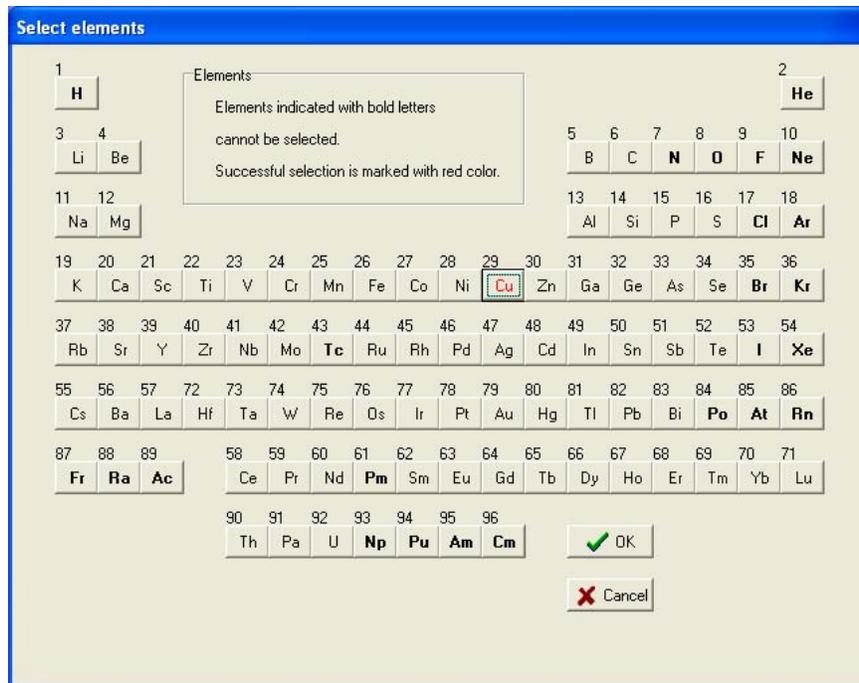


Figure 8. Screen for selecting an element (here Cu).

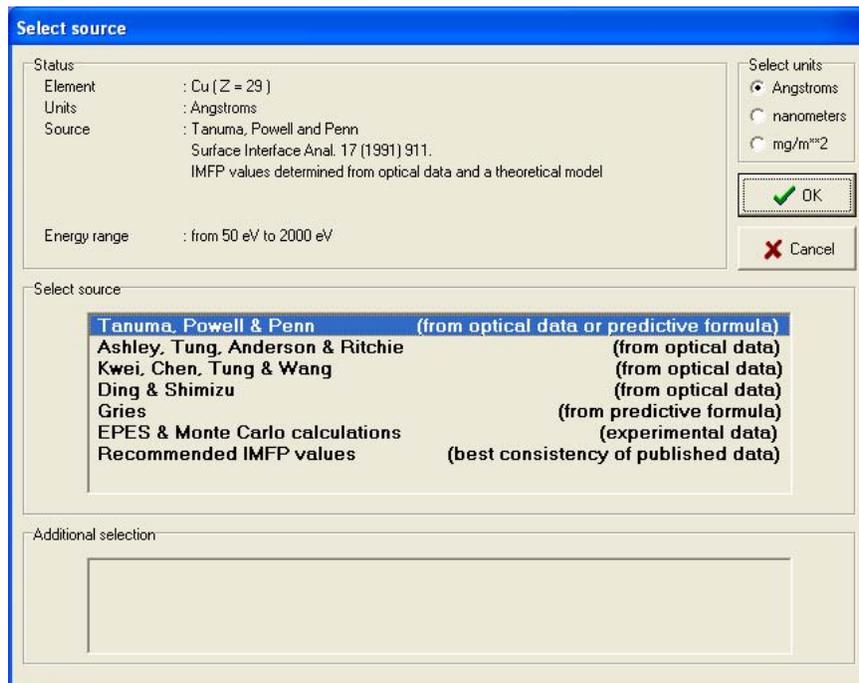


Figure 9. Sources of IMFP data for copper.

One of the data sources should then be selected. If experimental IMFP values are desired (i.e., IMFPs measured by elastic peak electron spectroscopy), an additional selection of a data source should be made in the bottom box of the screen. Further information concerning the selection(s) (the reference, the electron energy range for the IMFP data, and how the IMFP data were

obtained) appears in the status box. The user should also select the preferred IMFP units (Ångstroms, nanometers, or milligrams per square meter) in the box in the upper right of the screen (although units can be changed on later screens). The **OK** button should then be clicked.

Four types of data sources have been utilized to provide the IMFPs in the database:

1. IMFPs calculated from experimental optical data (for a group of elements and a small number of compounds). An analytic function has been fitted to calculated IMFPs for a particular material and data source to allow convenient interpolation [1,4].
2. IMFPs measured by elastic-peak electron spectroscopy (EPES) and the use of either Monte Carlo calculations or analytical theory (for a group of elements). An analytic function has been fitted to measured IMFPs for a particular material and data source to allow convenient interpolation [1,4].
3. IMFPs obtained from predictive formulae.
4. Recommended IMFPs (only for Ni, Cu, Ag, and Au) [1].

Further information on the sources of calculated, measured, and recommended IMFPs and the uncertainty of the IMFP data has been published elsewhere [1-4]. These references also contain a description of the procedures used to fit IMFPs that were calculated or measured at specific energies so that convenient interpolations can be made. The predictive formulae are described in Appendix A; for most applications, use of the TPP-2M equation of Tanuma *et al.* [5] is recommended.

For the example of Cu, seven separate data sources are shown in the screen of Figure 9. The first four of these are calculated IMFPs based on the work of the authors shown at the left of each line. For IMFPs from the work of Tanuma, Powell, and Penn [6], IMFPs are provided based on specific IMFP calculations for a selected element, if available, or otherwise from the predictive IMFP formula TPP-2M proposed by these authors [5]. If this formula has been utilized, information to this effect will be given on the screen for that element.

The following source in Figure 9 allows IMFPs to be calculated from the predictive IMFP equation (G-1 formula) of Gries [7].

The next line on the screen of Figure 9 indicates that measured IMFPs are available for Cu from EPES measurements and Monte Carlo calculations; selection of this line will lead to the appearance of six sources of data in the lowest box of Figure 8 from which the user should make a selection.

The last line on the screen of Figure 9 indicates that recommended IMFP values [1] are available for copper. The following screen (Figure 10) shows a graphical plot of calculated IMFPs for copper from Tanuma *et al.* [6] versus electron energy.

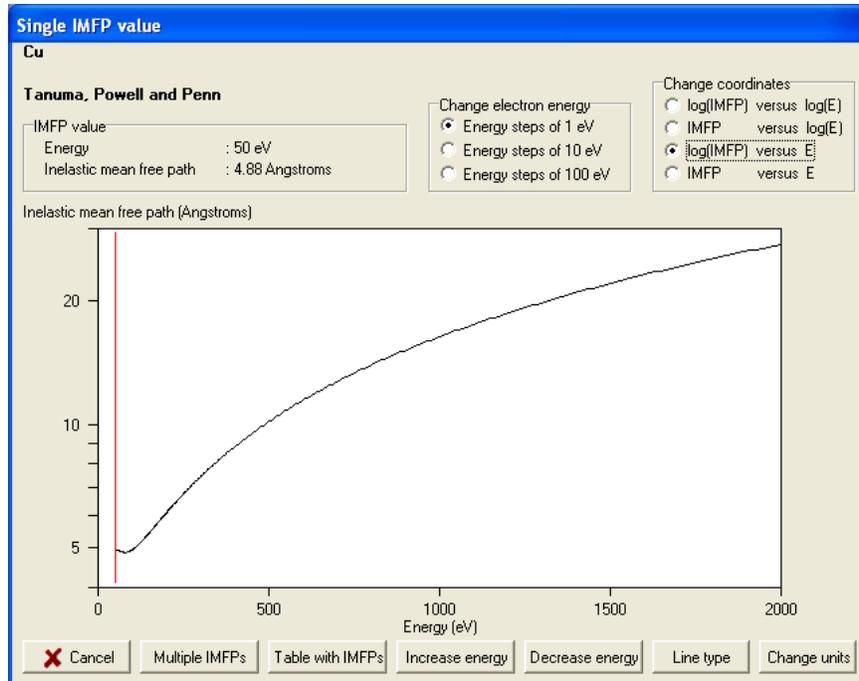


Figure 10. Graphical display of calculated IMFPs for copper (from Tanuma *et al.* [6]) as a function of electron energy.

The energy dependence of the cross section can be displayed in linear, semilogarithmic, or logarithmic coordinate systems; these coordinates are chosen with the buttons in the upper-right part of the screen. The IMFP units can be changed by clicking the **Change Units** button at the bottom-right of the screen, and the line type can be changed by clicking the **Line Type** button at the bottom of the screen. This plot provides a convenient means for showing the energy dependence of the IMFP. If it is desired to store or print a graphical plot such as that shown in Figure 10, a file with the IMFP data should be created with the Table with IMFP values option to be described shortly and then the Comparisons option of the main menu should be used to prepare a graphical display of the data in the file; this latter display can be printed and a file can be created for transfer to other applications.

An IMFP value for a particular energy can be found by clicking the cursor inside the plot at a position close to the desired energy. The IMFP and the chosen energy appear in the upper-left corner of the screen. The selected energy can be changed by clicking on the **Increase energy** or **Decrease energy** buttons; these changes will occur in steps of 1 eV, 10 eV, or 100 eV depending on the choice of button selected in the upper part of the screen. In this way, numerical IMFP values for particular electron energies of interest can be quickly found.

There are two additional methods by which numerical IMFP values for a particular material can be found and also stored. First, by clicking on the Multiple IMFPs button of the screen in Figure 10, the user can obtain IMFPs for specified electron energies. As an example, Figure 11 shows the screen that would appear if the silicon IMFP measurements of Gergely *et al.* [8] had been selected earlier; these IMFPs are derived from an analytic function fitted to the IMFP measurements [1].

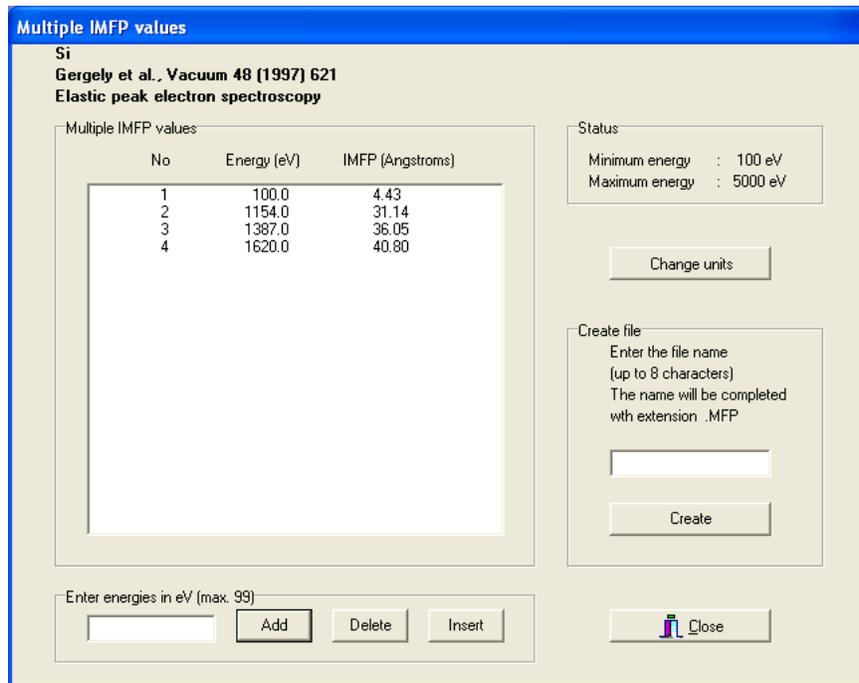


Figure 11. Example of multiple IMFP values from the measured IMFPs for silicon of Gergely *et al.* [8].

A series of electron energies can be entered into the box on the lower-left of the screen and the Add button clicked after each entry. These energies and the corresponding IMFPs will then appear in the center box of the screen. Entries in this box can be removed by selecting the relevant line(s) and clicking the Delete button. Similarly, new entries can be inserted above a selected line using the Insert button. The status box in the upper-right of the screen indicates the energy range of the original data; IMFPs can be obtained only for energies within this range. The IMFP units can be changed by clicking on the Change units button. Finally, a file can be created containing the indicated energies and IMFPs by entering a suitable file name in the box of the right-side of the screen and clicking the Create button. Such a file will be given the .MFP extension. A window will then appear on the screen indicating that the file has been successfully created; this window would show a diagnostic if, for example, an unsuitable file name had been chosen. This option is a convenient means of storing IMFPs at user-specified electron energies for a selected material and data source.

Second, a Table can be created containing IMFPs for regularly spaced electron energies within the energy range of the original data source. Figure 12 shows the screen that would appear if the Table with IMFPs button in Figure 10 had been clicked and if measured IMFPs for silicon from Gergely *et al.* [8] had been previously selected.

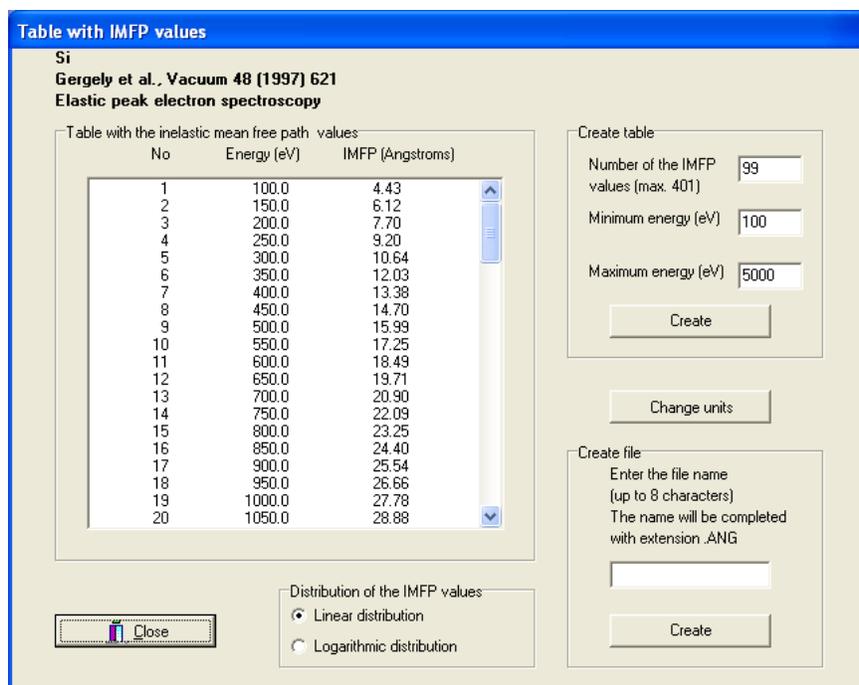


Figure 12. Table with IMFP values derived from the measured IMFPs for silicon of Gergely *et al.* [8].

The number of IMFP values in the Table can be selected by the user in the box at the upper-right of the screen; the default value is 401 (the maximum number). The user can also choose to have the energy values in the Table distributed uniformly on either linear or logarithmic scales by selecting the appropriate button on the lower part of the screen. Clicking on the **Create** button in the upper-right of the screen will then create the Table in the center of the screen. The IMFP units can be changed as before by clicking on the **Change units** button. Finally, a file can be created containing the Table of energies and IMFPs by entering a suitable file name and clicking on the Create button in the lower-right of the screen. Files of this type are given extensions of .ANG, .NAN, or .MGM depending on whether the IMFP units are Angstroms, nanometers, or milligrams per square meter, respectively. This option is a convenient means of storing IMFP data for a selected material and data source over the energy range of the original data (shown at the upper-right of the screen). This file can be later used to create a graphical display of the IMFP data (e.g., for comparisons, printing, or transfer to other applications).

Clicking on the **Close** button in Figs. 11 and 12 will return the user to the main menu. It is then possible to go directly to screens for obtaining a single IMFP value (Figure 10), multiple IMFP values (Figure 11), or a Table with IMFP values (Figure 12) for the previously selected element and data source using the submenu shown in Figure 3(a).

Inorganic Compounds

(Second option of the Database option on the main menu)

The user can choose to obtain calculated IMFPs for a limited number of inorganic compounds or to derive IMFPs from predictive formulae (Figure 3(b)). If the first choice is made, the screen of

Figure 13 appears in which four sources of calculated IMFPs are shown in the center part of the screen.

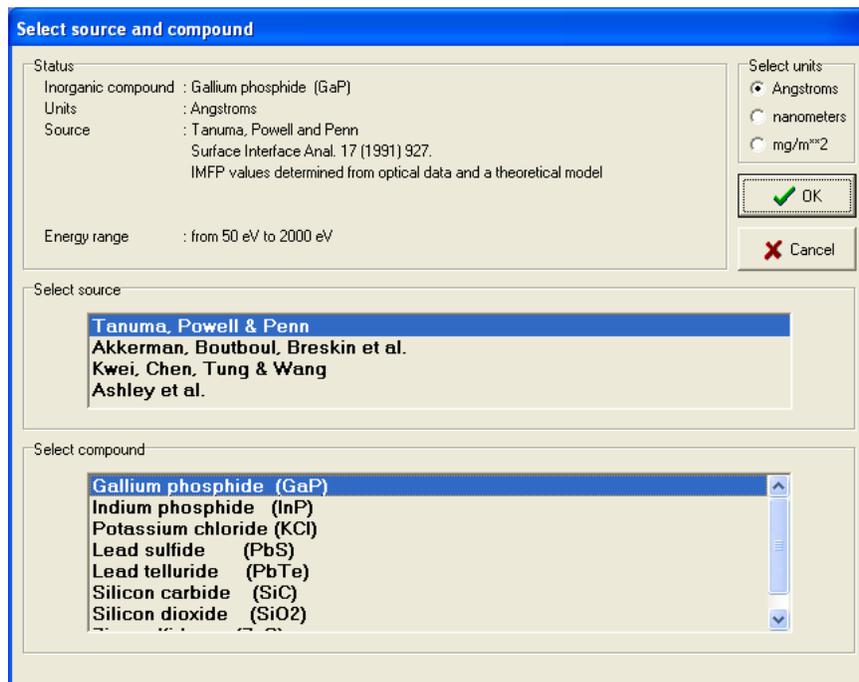


Figure 13. Screen to select source and compound to obtain calculated IMFPs for inorganic compounds.

If one of those sources is selected, the compounds for which calculated IMFPs are available appear in the lower part of the screen. After a compound is selected (and, if desired, the IMFP units changed using the box at the upper-right of the screen), the **OK** button is clicked and a series of screens similar to Figs. 10, 11, and 12 will then appear depending on whether the user wishes to obtain an IMFP value for a single electron energy, multiple IMFP values, or a Table of IMFP values as described for Elements in the previous section.

If the second choice is made, a Periodic Table of the elements similar to Figure 8 appears (but now the gaseous elements are not shown in bold). At least two elements should be selected by clicking on the appropriate boxes. After clicking the **OK** button, a screen similar to Figure 14 appears.

The name of the compound should be entered in the box in the upper-left of the screen. The stoichiometry coefficients for each element in the compound should then be entered in the next lower box.

IMFPs from predictive formulae

Enter the name of the inorganic compound
(the name should not exceed 55 characters)

Gallium phosphide (GaP)

Select predictive formula

TPP-2M equation
 Gries (G1 equation)

Select units

Angstroms
 Nanometers
 mg/m²

Enter density (g/cm³)

4.13

Enter the stoichiometry coefficients

Element	Atomic number	Stoichiometry coefficient
P	15	1.000
Ga	31	1.000

P 15 1.000

Add

Enter the number of valence electrons per molecule, Nv

8

Enter the band-gap energy, Eg (eV)

2.24

Comment

To continue, all the input parameters listed here must be introduced

OK

Cancel

Figure 14. Screen used to obtain IMFPs from predictive formulae for inorganic compounds.

The user can choose to obtain IMFP values from the predictive TPP-2M equation of Tanuma *et al.* [5] or the predictive G-1 equation of Gries [7] using one of the buttons in the top-right of the screen; these equations are described in Appendix A. If the TPP-2M equation is selected, values for the density, number of valence electrons per molecule, and bandgap energy should be entered into the appropriate boxes; information on the latter two parameters is given in Appendix A. If the G-1 equation is selected, only the density value should be entered. The IMFP units can be changed, if desired, using the buttons on the right side of the screen. After clicking OK, screens similar to Figs. 10, 11, and 12 will appear. It is possible to go directly to the desired screens from the main menu after a data source and compound have been selected using the submenu options shown in Figure 3(b).

Further information on the sources of calculated IMFPs for the inorganic compounds and on their uncertainties has been published elsewhere [1-4].

Organic Compounds (Third option of the Database option on the main menu)

Similar choices are made to obtain IMFPs for organic compounds as described above for inorganic compounds, as in Figure 3(c). Figure 15 shows the screen that indicates sources of calculated IMFPs for organic compounds and, for the selected source, the compounds for which IMFPs are available.

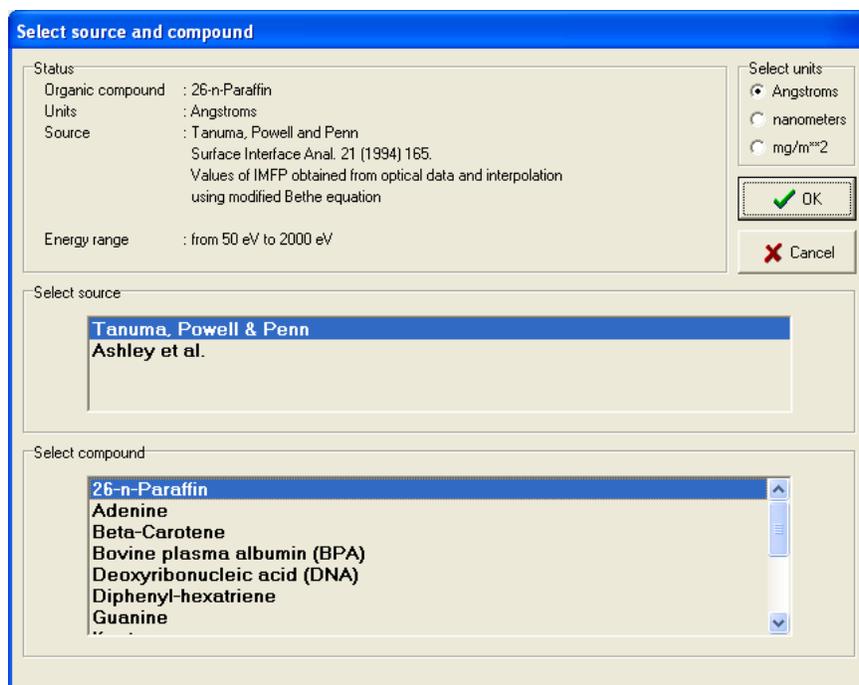


Figure 15. Screen to select source and compound to obtain calculated IMFPs for organic compounds.

File Management (Second option of the main menu)

With this option, a user can save files created in the present session to another directory for permanent storage, delete files from the database directory, print files containing IMFP data, print figures showing displays of IMFP data as a function of electron energy, and load files containing IMFP data or figures that were created in earlier sessions and stored in another directory (Figure 4). These options will be described in turn.

Save Created Files (First option of the File Management option on the main menu)

Files containing IMFP values are created by the database (as described above) as text files in the directory in which the database is located (default C:\PROGRAM FILES\NIST\IMFPWIN). The files created by the Table with the IMFP values option have extensions of .ANG, .NAN, or .MGM (for which the IMFPs are in units of Ångstroms, nanometers, or milligrams per square meter, respectively) while the files created by the Multiple IMFP values option have the .MFP extension. Files containing IMFP figures are created by the Comparisons option (see below) and have the .BMP extension.

The Save files option allows the user to save files in the database directory to any other directory for permanent storage. Figure 16 shows an example of a screen for this option.

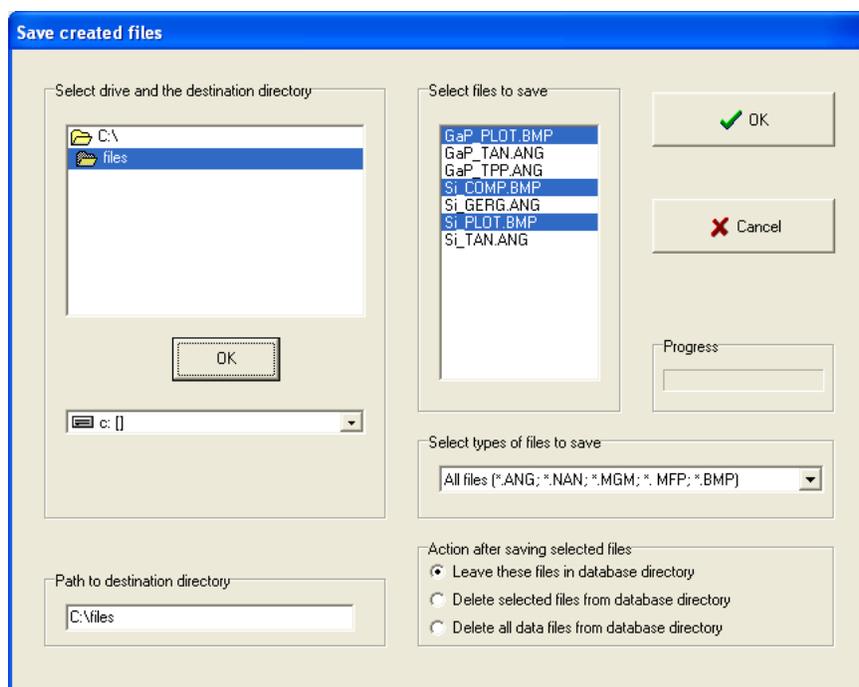


Figure 16. Example of saving three files from the database directory to the C:\FILES directory.

The center panel shows illustrative data files in the database directory; if desired, files with particular extensions can be selected for display using the box on the right side of the screen. The file(s) to be saved should be selected by clicking on the file name(s) (and simultaneously pressing the Shift key or the Ctrl key if multiple selections are desired). The destination directory for the saved files is selected in the panel located in the lower-left corner of the screen; in Figure 16, the directory C:\FILES has been selected as the destination directory for three selected files. The user then selects one of the three buttons in the lower-right corner of the screen to indicate whether the selected files should also be retained in the database directory after the Save files operation, whether these files should be removed from this directory, or whether all data files in the directory should be removed. The **OK** button should then be clicked to save the designated files. Appendix B gives an example of the content and format of a saved text file.

Delete Files

(Second option of the File Management option on the main menu)

Data files created during the present session or during previous sessions can be deleted with this option. Figure 17 shows an example of this option.

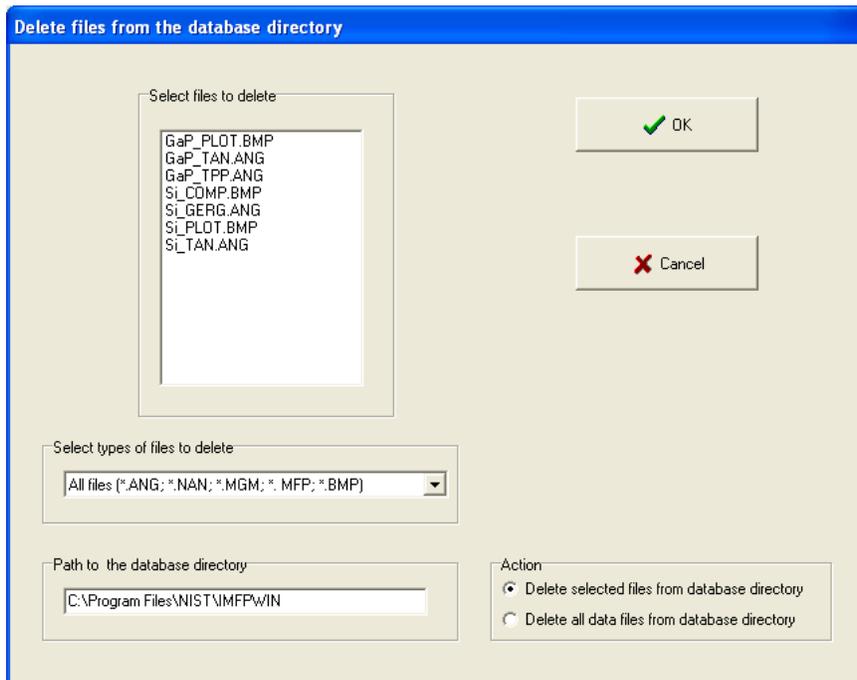


Figure 17. Screen illustrating deletion of a file from the database directory.

The user should initially select the directory from which files are to be removed; by default, the database directory is selected, as shown in Figure 17. It is possible to display files with selected extensions using the middle box on the left of the screen. The user then selects one or more files for deletion from the list. If desired, all data files in the database directory can be deleted by choosing the second button in the lower-right of the screen. Deletion of the selected files occurs after the **OK** button is clicked.

Print Files

(Third option of the File Management option on the main menu)

IMFP files created by the database (i.e., those with .ANG, NAN, MGM, and MFP extensions) are text files and can be opened and printed by common word-processing software. These files can also be printed with this option of the database. A screen similar to Figure 18 appears and, if desired, the user can select files with a particular extension for listing.

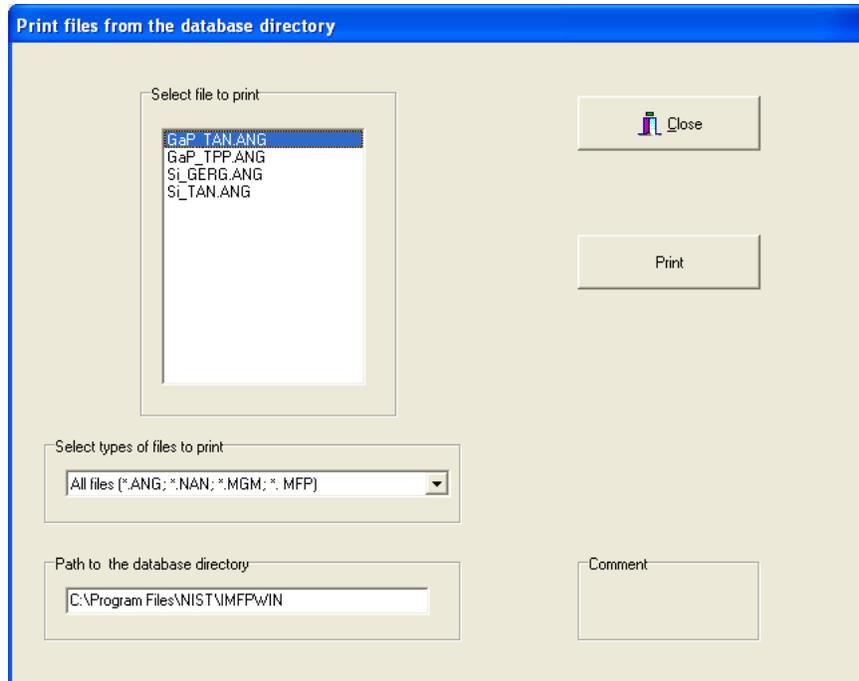


Figure 18. Screen illustrating selection of an IMFP file from the database directory for printing.

Unlike the previous file-management options, the user can only select a single file for printing at a time. Printing is initiated by clicking the **Print** button. If a user wishes to print files stored in other directories, these files can be loaded into the database directory using the Load files option described below. Appendix B contains an example of a printed file.

Print Figures (Fourth option of the File Management option on the main menu)

Files with figures created by the Comparisons option of the database (see below) have the .BMP extension and can be inserted into documents produced by common word-processing software. These files can also be printed with this option of the database. A screen similar to Figure 19 appears that lists files with the .BMP extension in the database directory on the right side of the screen.

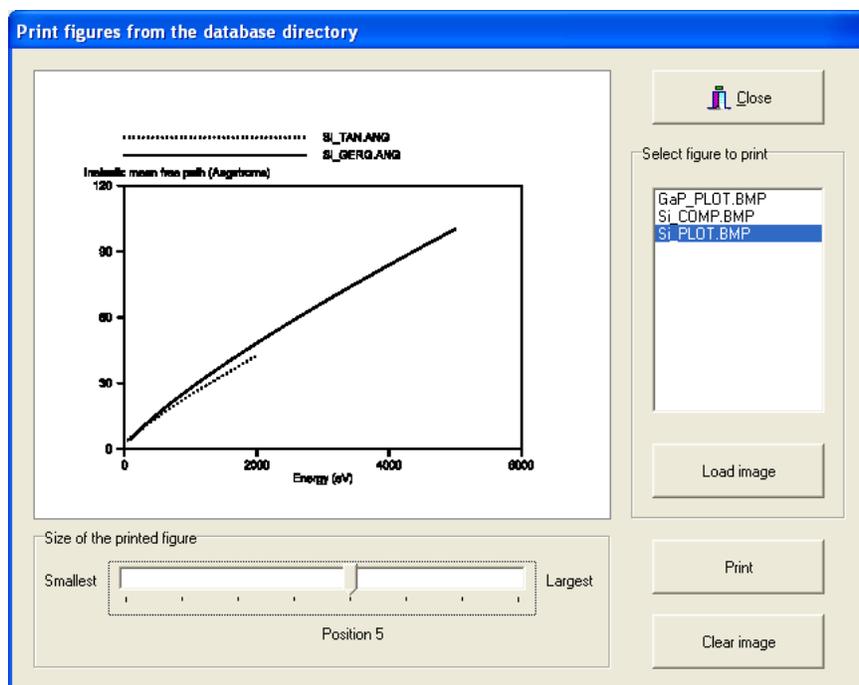


Figure 19. Screen illustrating selection of a figure from the database directory for printing.

A file can be selected and, after clicking the **Load image** button, the figure appears in the center of the screen. This figure can be printed in one of eight sizes by moving the pointer in the lower part of the screen with the mouse. The printed sizes are approximately 5 cm x 4 cm, 7 cm x 5 cm, 8.5 cm x 6.5 cm, 10 cm x 7.5 cm, 11.5 cm x 9 cm, 13 cm x 10 cm, 14.5 cm x 11 cm, and 16 cm x 12 cm for pointer positions 1, 2, 3, 4, 5, 6, 7, and 8, respectively. Clicking the **Print** button initiates printing. Files with figures that are stored in other directories can be loaded into the database directory using the Load files option.

Load Files

(Fifth option of the File Management option on the main menu)

With this option, it is possible to transfer files to the current database directory (default: C:\PROGRAM FILES\NIST\IMFPWIN) that had been saved previously to other directories. An example of this option is shown in Figure 20.

In this example, the directory C:\FILES has been selected as the source directory in the upper-left box on the screen. It is possible to load files with the .ANG, .NAN, .MGM, .MFP, and .BMP extensions, and listings of files with selected extensions can be chosen using the box in the lower-right of the screen. One or more of the files listed in the upper part of the screen can be selected and then loaded into the database directory by clicking **OK**.

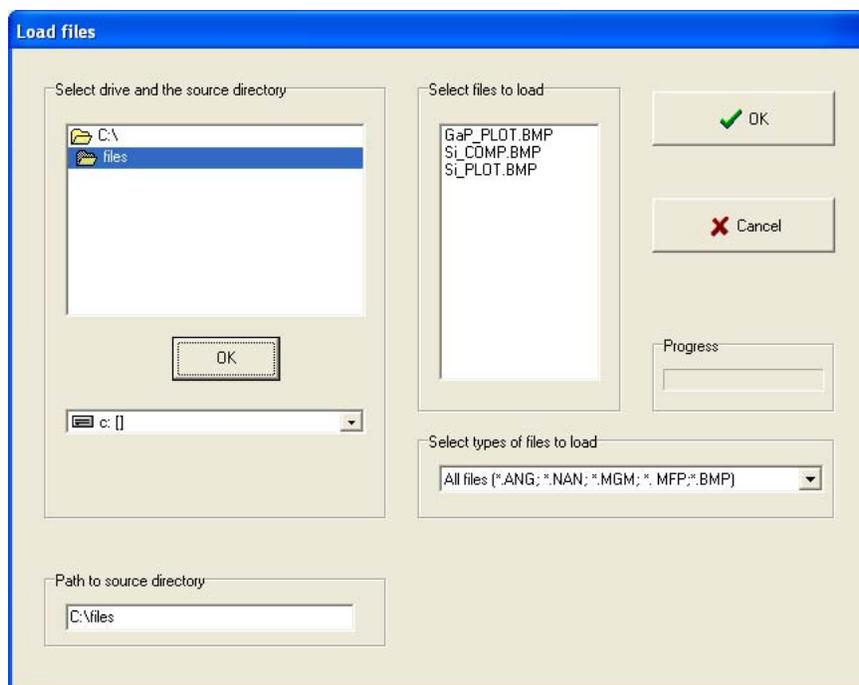


Figure 20. Example of loading a file from the C:\FILES directory to the database directory; in this example, files with a .BMP extension are listed.

Comparisons (Third option of the main menu)

This option is useful for making graphical comparisons of IMFP data from different sources for the same material or for comparing IMFP data from different materials. The option is also useful for creating a graphical display with a single set of IMFP data. These graphical displays can be stored or printed for later use.

Files containing IMFP data are needed for use of this option. These files can be created from IMFPs provided by the database for any material using the Multiple IMFP values or Table with IMFP values options described above for the Elements option of the Database option in the main menu. The IMFP data to be compared must be in the same units; that is, the IMFPs to be compared will be in files with extensions of .ANG, .NAN, and .MGM for IMFPs expressed in Ångstroms, nanometers, and milligrams per square meter, respectively. Alternatively, files with these extensions that were created in previous sessions and stored in other directories can be loaded into the database directory using the Load files option described above.

On selection of this option, the user will choose to compare IMFPs only from the database or to compare IMFPs from the database and other sources (Figure 5). In the latter case, comparisons are made with IMFP data from other sources (e.g., recent publications) that are entered by the user. These two options will now be described.

Inelastic Mean Free Paths from the Database Only

Figure 21 shows an example of a screen that appears when this option is chosen.

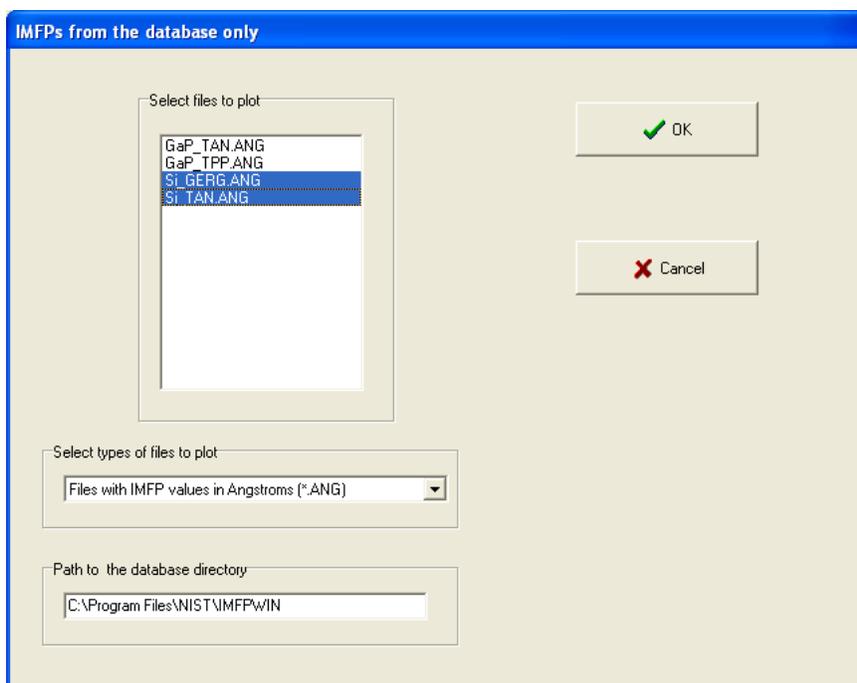


Figure 21. Screen showing selection of two files from the database directory with IMFP data to be compared.

Files with IMFPs in the desired units can be listed according to their extensions using the box in the middle-left of the screen. Up to four files can be selected for comparison at a time. The **OK** button should then be clicked. Figure 22 is an example of a graphical comparison of IMFPs calculated for silicon by Tanuma *et al.* [6] and of IMFPs measured for silicon by Gergely *et al.* [8].

Linear, logarithmic, or semi-logarithmic display coordinates can be selected using buttons on the upper-right of the screen. The line type on the display can be varied by clicking the **Line type** button, and the display can be printed by clicking the **Print** button. A file containing the display can be created by clicking the **Create file** button; a window will then appear in which the user can enter a suitable file name. This file will have the .BMP extension.

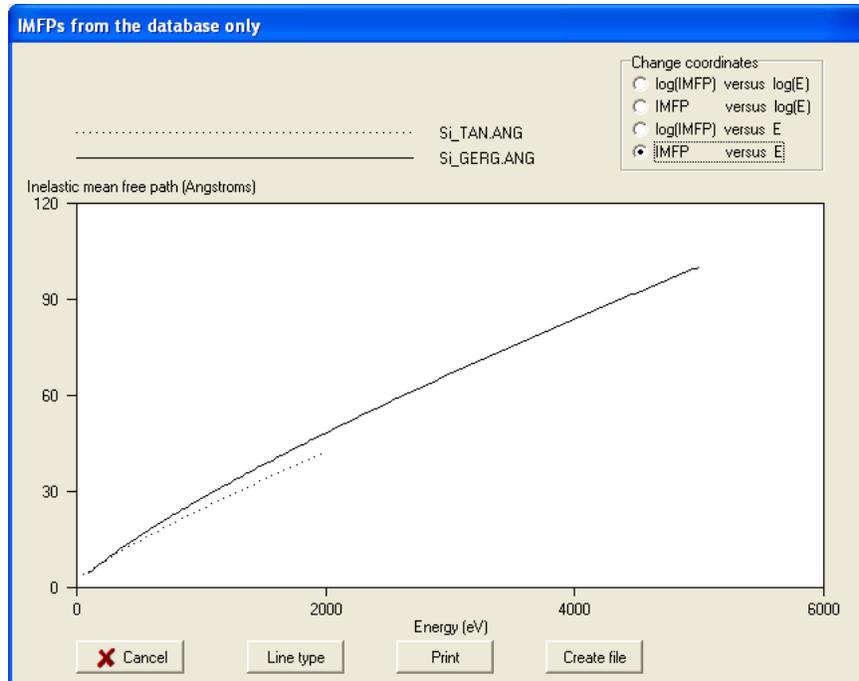


Figure 22. Screen showing comparison of IMFPs for silicon from two data files. The dotted line shows IMFPs calculated by Tanuma *et al.* [6] and the solid line shows IMFPs measured by Gergely *et al.* [8].

Inelastic Mean Free Paths from Other Sources and the Database

If this option is chosen, a screen similar to Figure 23 appears. With this screen, one or more files in the database directory can be selected as in Figure 21. In addition, the user can enter electron energies (in eV) and corresponding IMFP values (in the same units as the IMFP data in the selected files) in the boxes on the right side of the screen; on clicking the **Add** button, these entries will be transferred to the summary box above. If desired, a line on this box can be selected and then removed by clicking the **Delete** button. When data entry is complete, the OK button should be clicked, and a screen similar to Figure 24 will appear. This screen shows IMFPs for silicon from the same sources as in Figure 22. The open circles in Figure 24 are effective attenuation length (EAL) values for silicon that were measured by Ebel *et al.* [7] (and which were entered on the screen of Figure 23). As expected, the EALs are smaller than the corresponding IMFPs [8].

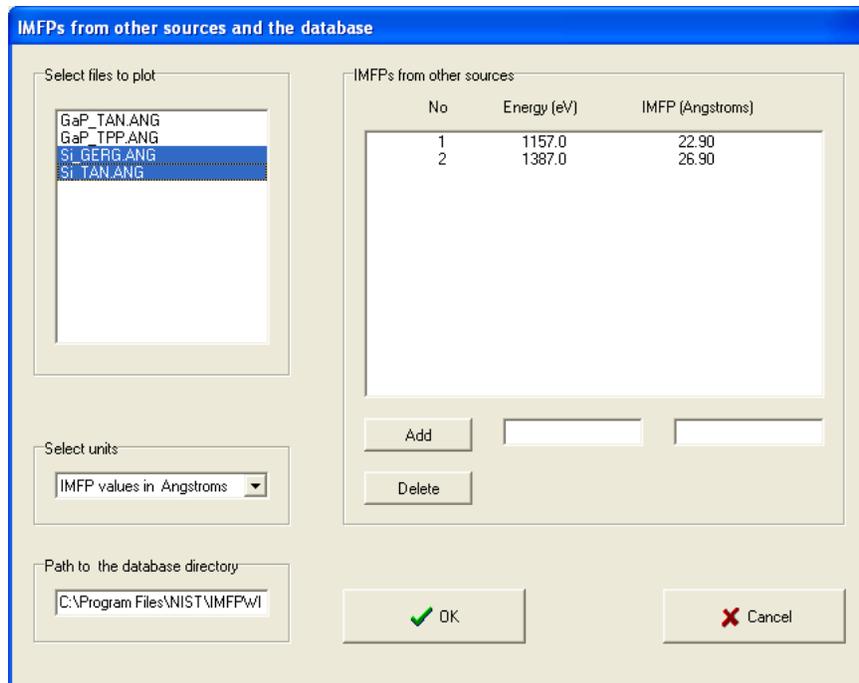


Figure 23. Example of selection of files for comparison of IMFP data from the selected files with IMFP data entered by the user.

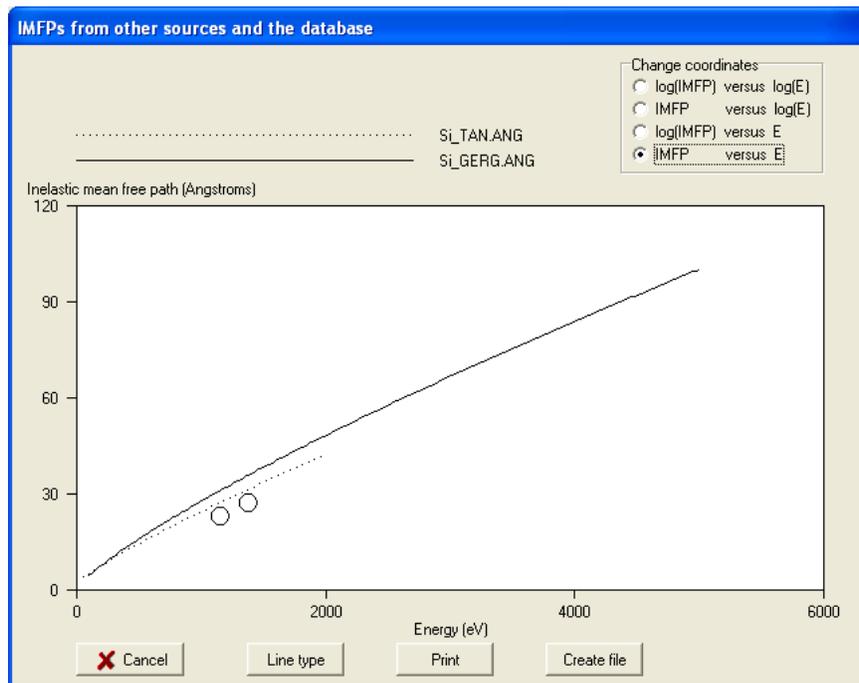


Figure 24. Screen showing IMFPs for silicon from the two data files shown in Figure 23. The dotted line shows IMFPs calculated by Tanuma *et al.* [6] and the solid line shows IMFPs measured by Gergely *et al.* [8]. The open circles show effective attenuation lengths for silicon measured by Ebel *et al.* [10].

V. UNCERTAINTIES OF CALCULATED, MEASURED, AND PREDICTED INELASTIC MEAN FREE PATHS

Detailed evaluations of the uncertainties of IMFPs calculated from experimental optical data, IMFPs measured by elastic-peak electron spectroscopy (EPES), and IMFPs obtained from predictive formulae have been published [1-4,11]. We will give here a brief summary of information from these evaluations. The most detailed analysis was of calculated and measured IMFPs for seven elemental solids (Al, Si, Ni, Cu, Ge, Ag, and Au) for which there were calculated IMFPs from at least two independent sources and measured IMFPs from at least two independent sources [1].

Consistency of Calculated Inelastic Mean Free Paths

It was convenient to compare calculated IMFPs for a particular material from a particular source over the available energy range with IMFP values obtained from a function fitted to calculated IMFPs from all available sources for that material [1]. Two measures of deviation of individual IMFP values from the fitted IMFPs were employed. First, the average root-mean-square deviation *RMS* of the individual IMFPs from the fitted IMFPs was found to be 0.89 Å for the group of seven elemental solids [1]. Second, the average of the mean percentage deviations *R* for each element of the individual IMFPs from the fitted IMFPs was found to be 4.4 % [1]. Similar values of *RMS* and *R* were found in similar evaluations of calculated IMFPs for Fe, Al₂O₃, SiO₂, KCl, poly(butene-1-sulfone), polyethylene, and polystyrene [4]. The values of *RMS* and *R* for the seven elements indicate the variability in IMFPs that can be found from the use of different sets of optical data and different technical approaches [1].

Consistency of Measured Inelastic Mean Free Paths

For the same group of seven elemental solids, a similar comparison was made of measured IMFPs for a particular material from a particular source over the available energy range with IMFP values obtained from a function fitted to measured IMFPs from all available sources for that material [1]. Values of *RMS* and *R* were again computed to describe the variability of the measured IMFPs for each solid with respect to the fitted IMFPs. For the seven elemental solids, the average value of *RMS* was 3.00 Å and the average value of *R* was 13.2 % [1]; these values are about three times larger than the corresponding values for the calculated IMFPs. Similar values of *RMS* and *R* were found in comparisons of measured IMFPs for Fe, Mo, W, and Pt [4]. The values of *RMS* and *R* for the seven elements are a measure of the uncertainties of IMFP measurements by EPES [1].

Consistency of Calculated and Measured Inelastic Mean Free Paths

A similar comparison has been made of the measured IMFPs for the seven elemental solids with the corresponding calculated IMFPs [1]. It was convenient to compare the measured IMFPs for each element to a function fitted to all of the calculated IMFPs for that element. Values of *RMS* and *R* were again calculated to describe the deviations of the measured IMFPs about the fitted IMFPs. For the seven elemental solids, the average value of *RMS* was 4.56 Å and the average value of *R* was 17.4 % [1]. Similar values of *RMS* and *R* were found in comparisons of measured IMFPs for Fe, Mo, W, and Pt with functions fitted to the calculated IMFPs for these elements [2]. Although the values of *RMS* and *R* found in the comparisons of measured and calculated IMFPs are much greater than the corresponding values found in the comparison of calculated

IMFPs from different sources, the precision of IMFP measurement in a particular laboratory is generally sufficient to show that the energy dependence of the measured IMFPs is close to that expected from the IMFP calculations [1,4].

Recommended Inelastic Mean Free Paths

In the comparisons of the calculated IMFPs for each of the seven elements, comparisons of the measured IMFPs for those elements, and comparisons of the calculated and measured IMFPs for the same elements, it was found that the values of *RMS* and *R* for Ni, Cu, Ag, and Au were appreciably less than the corresponding average values for the group of seven elements [1]. The database contains “recommended IMFPs” for Ni, Cu, Ag, and Au that were derived from a function fitted to the calculated IMFPs for each element [1].

Uncertainties of Calculated and Measured Inelastic Mean Free Paths

In the comparisons of calculated and measured IMFPs described above for the group of seven elements, the values of *RMS* and *R* are considered to be indications of the uncertainties in the calculations and measurements, respectively. These values of *RMS* and *R*, however, should be considered as lower limits to the uncertainty because it has not been possible to quantify potential sources of systematic error in the calculations and measurements [1-3]. In the absence of more detailed knowledge of the systematic errors in the IMFP calculations and measurements, the average value of $RMS = 4.56 \text{ \AA}$ found in the comparison of measured IMFPs with the function fitted to the calculated IMFPs for each of the seven elements and the corresponding average value of $R = 17.4 \%$ will be considered as reasonable estimates of the IMFP standard uncertainty.

This discussion of uncertainties has been based on an evaluation of calculated and measured IMFPs for seven solid elements [1]. There is no known reason for the uncertainties in IMFPs of other materials to be substantially different. Measured IMFPs for non-elemental solids, however, may have additional uncertainty due to the need to determine the surface composition over the depth probed by EPES if there is reason to believe that this could be different from the bulk composition [1].

For some elements and compounds, the database contains more than one source of calculated or measured IMFPs. In general, it has not been possible to quantify the uncertainties in individual IMFP measurements or calculations. Until this can be done, no guidance can be given to a preferred source of data. The “recommended IMFPs” should nevertheless be used for Ni, Cu, Ag, and Au. For these four elements, calculated and measured IMFPs from other sources are also provided so that users can access these data if they wish to (or if future analyses show that IMFPs from particular sources have a lower uncertainty).

There is an additional source of uncertainty in IMFPs from the database arising from the use of analytical functions to fit the calculated and measured IMFPs from each source so that interpolations could be made. Information on this uncertainty is given elsewhere [1,4].

Uncertainties of Inelastic Mean Free Paths from Predictive Formulae

IMFPs can be obtained conveniently from two predictive formulae in the database, the TPP-2M equation of Tanuma *et al.* [5] and the G-1 equation of Gries [7]. These formulae can be used to obtain IMFPs in materials for which no IMFP calculations or measurements have been made. These two equations are described in Appendix A.

Information on uncertainties of IMFPs from the two equations will now be presented.

TPP-2M Equation of Tanuma, Powell, and Penn

Tanuma *et al.* [5] derived their TPP-2M equation from an analysis of their calculated IMFPs for electrons of 50 eV to 2000 eV energy in a group of 27 elements [6] and a group of 14 organic compounds [5]. This equation is based on the Bethe equation [12] for inelastic electron scattering in matter but with modifications suggested by Inokuti [13] and Ashley [14] to describe the IMFP dependence on energy for energies less than 200 eV.

Comparison of IMFPs from the TPP-2M equation with those directly calculated from optical data showed average RMS deviations of 10.2% for the group of 27 elements, 8.5 % for the group of 14 organic compounds, and 18.9% for the group of 15 inorganic compounds [5]. These deviations were considered to be satisfactorily small on account of the similar uncertainty of the optical data used in the IMFP calculations and the empirical nature of the modifications to the Bethe equation. The larger deviations found for the inorganic compounds was expected because the optical data for these compounds had greater sum-rule errors than for the other materials [5,15].

Comparisons of IMFPs calculated from the TPP-2M equation for Ni, Cu, Ag, and Au with the corresponding recommended IMFPs for these elements show satisfactory agreement [4]. The average value of *RMS* between IMFPs from the TPP-2M equation and the corresponding recommended IMFPs was 0.90 Å and the corresponding value of *R* was 10.9 % [4].

The uncertainties of IMFPs obtained from the TPP-2M equation can be expressed in two ways depending on the intended application of the data. If, for example, IMFPs for two materials are to be compared, then the standard uncertainty of each is estimated from the comparison with the recommended IMFPs to be 0.90 Å or 10.9 %. If absolute values of IMFPs are required, the standard uncertainty will be the quadrature sum of one of these values and the corresponding uncertainty found in the comparison of measured and calculated IMFPs (4.56 Å and 17.4% for *RMS* and *R*, respectively). This combined standard uncertainty is thus estimated to be 4.7 Å or 20.5 %.

There is one additional source of uncertainty in the use of the TPP-2M equation. For some elements, it is not clear whether the parameter N_v should be simply the number of valence electrons, as defined in Appendix A, or whether this number should be increased to include the number of core electrons with binding energies of less than about 30 eV [6,16]. For some elements (listed in Table A.1), N_v has been increased to include these shallow core electrons but for others the core electrons have been excluded. In some cases, the inclusion or exclusion of the shallow core electrons does not lead to changes of more than 20 % in the IMFPs calculated from the TPP-2M equation but larger changes can be found for other elements [17].

G-1 Equation of Gries

Gries [7] developed his G-1 equation from an analysis of the calculated IMFPs of Tanuma *et al.* [5,6,15] over the 200 eV to 2000 eV range and an atomistic model of inelastic electron scattering. The G-1 equation has a different dependence on material parameters than the TPP-2M equation of Tanuma *et al.* At an energy of 2 keV, the average deviations between IMFPs from the G-1 equation and IMFPs of Tanuma *et al.* were similar in magnitude to those reported by Tanuma *et al.* [5] for their TPP-2M equation (although it should be noted that the comparisons of Tanuma *et al.* were made over the 50 eV to 2000 eV energy range).

Tanuma *et al.* [11] have analyzed the Gries model and have pointed out some important limitations. Although the G-1 equation provides useful estimates of IMFPs for many elements and compounds, there can be substantial deviations (of up to about 50%) for a few of the materials that have been examined to date. Since there is presently no explanation for these deviations, it is believed that the TPP-2M equation has greater general reliability [11]. Although use of the G-1 equation requires knowledge of just one material parameter (the specimen density), it is recommended that IMFPs be determined from this equation only if a user has reason to believe that the TPP-2M equation will not give satisfactory results.

REFERENCES

1. Powell, C. J., and Jablonski, A., *J. Phys. Chem. Ref. Data* 28, 19 (1999).
2. *Nucl. Instr. Meth. Phys. Res. A* 601, 54 (2009).
3. Powell, C. J., and Jablonski, A., *J. Electron Spectrosc. Rel. Phenom.* 178-179, 331 (2010).
4. Powell, C. J., and Jablonski, A., *Surf. Interface Anal.* 29, 108 (2000).
5. Tanuma, S, Powell, C. J., and Penn, D. R., *Surf. Interface Anal.* 21, 165 (1994).
6. Tanuma, S, Powell, C. J., and Penn, D. R., *Surf. Interface Anal.* 17, 911 (1991).
7. Gries, W. H., *Surf. Interface Anal.* 24, 38 (1996).
8. Gergely, G., Konkol, A., Menyhard, M., Lesiak, B., Jablonski, A., Varga, D., and Toth, J., *Vacuum* 48, 621 (1997).
9. Ebel, M. F., Ebel, H., Hofmann, A., and Svagera, R., *Surf. Interface Anal.* 22, 51 (1994).
10. Jablonski, A., and Powell, C. J., *J. Electron Spectrosc. Relat. Phenom.* 100, 137 (1999); *ibid.* 107, 201 (2000).
11. Tanuma, S, Powell, C. J., and Penn, D. R., *Surf. Interface Anal.* 25, 25 (1997).
12. Bethe, H., *Ann. der Physik* 5, 325 (1930).
13. Inokuti, M., *Rev. Mod. Phys.* 43, 297 (1971).
14. Ashley, J. C., *J. Electron Spectrosc. Relat. Phenom.* 46, 199 (1988).
15. Tanuma, S, Powell, C. J., and Penn, D. R., *Surf. Interface Anal.* 17, 927 (1991).
16. Tanuma, S, Powell, C. J., and Penn, D. R., *Surf. Interface Anal.* 11, 577 (1988).
17. Tanuma, S, Powell, C. J., and Penn, D. R. (to be published).
18. Seah, M. P., and Gilmore, I. S., *Surf. Interface Anal.* 26, 908 (1998).
19. Seah, M. P. (private communication).
20. Smith, D. M., Gallon, T. E., and Matthew, J. A. D., *J. Phys. B* 7, 1255 (1974).
21. Netzer, F. P., and Matthew, J. A. D., *Rep. Prog. Phys.* 49, 621 (1986).
22. *American Institute of Physics Handbook*, D. E. Gray, ed. (McGraw-Hill, New York, 1963), p. 9-22.
23. Ashcroft, N. W., and Mermin, N. D., *Solid State Physics* (Holt, Rinehart and Winston, 1976), p. 566.
24. Kittel, C., *Introduction to Solid State Physics*, sixth edition (John Wiley, New York, 1986), p. 185.
25. Wolfe, C. M., Holonyak, J., and Stillman, G. E., *Physical Properties of Semiconductors* (Prentice-Hall, Englewood Cliffs, 1989).
26. *CRC Handbook of Chemistry and Physics*, 77th edition, D. R. Lide, ed. (CRC Press, Boca Raton, 1996), pp. 12-94–12-98.
27. Tanuma, S, Powell, C. J., and Penn, D. R., *Surf. Interface Anal.* 20, 77 (1993).
28. Coplen, T. B., *Pure Appl. Chem.* 68, 2339 (1996).
29. *CRC Handbook of Chemistry and Physics*, 77th edition, D. R. Lide, ed. (CRC Press, Boca Raton, 1996), pp 4-37–4-98.
30. *CRC Handbook of Chemistry and Physics*, 77th edition, D. R. Lide, ed. (CRC Press, Boca Raton, 1996), pp 3-3–3-330.

Appendix A

PREDICTIVE FORMULAE FOR ELECTRON INELASTIC MEAN FREE PATHS

IMFPs can be obtained conveniently from two predictive formulae in the database, the TPP-2M equation of Tanuma *et al.* [5] and the G-1 equation of Gries [7]. These formulae can be used to obtain IMFPs in materials for which no IMFP calculations or measurements have been made. Information on the uncertainties of IMFPs from these two formulae is given in Section V.

These predictive formulae will now be described in turn. Information on atomic weights and elemental densities is given in the final section.

TPP-2M Equation of Tanuma, Powell, and Penn

Tanuma *et al.* [5] proposed the following equations for the calculation of the IMFP λ (in Ångstroms) as a function of electron energy E (in eV) and various material parameters:

$$\lambda = \frac{E}{E_p^2[\beta \ln(\gamma E) - (C/E) + (D/E^2)]} \quad (\text{A.1})$$

where

$$\beta = -0.10 + 0.944/(E_p^2 + E_g^2)^{1/2} + 0.069\rho^{0.1} \quad (\text{A.2})$$

$$\gamma = 0.191\rho^{-0.50} \quad (\text{A.3})$$

$$C = 1.97 - 0.91U \quad (\text{A.4})$$

$$D = 53.4 - 20.8U \quad (\text{A.5})$$

$$U = N_v\rho/M = E_p^2/829.4 \quad (\text{A.6})$$

and $E_p = 28.8 (N_v\rho/M)^{1/2}$ is the free-electron plasmon energy (in eV), ρ is the density (in g cm⁻³), N_v is the number of valence electrons per atom (for an element) or molecule (for a compound), M is the atomic or molecular weight, and E_g is the bandgap energy (in eV). Equations (A.1) through (A.6) are collectively known as the TPP-2M equation.

Table A.1 shows recommended elemental values for the parameter N_v in the TPP-2M equation. During the development of the TPP-2M equation, there was ambiguity in the choice of a value of N_v for elements in which there were core-levels with binding energies less than about 30 eV [6,16,17]. Measurements of Auger-electron yields for many solid elements by Seah and Gilmore [18], however, have given experimental guidance on the appropriate choice of N_v for many elements. For the rare-earth elements, these authors recommended that the 4f electrons should be excluded in the count for N_v . In more recent work from the same group, however, the

recommended choices for the rare-earth elements have been revised [19] to include the 4f electrons but the details of the analysis have not been published. Comparisons of IMFPs calculated from optical data for Gd, Tb, and Dy with IMFPs obtained from the TPP-2M equation and various values of N_v nevertheless indicate that the 4f electrons should be excluded [17]. This conclusion is supported by an analysis of the energy-loss function for these three elements and the expectation that the 4f electrons do not contribute substantially to the energy-loss function for energy losses less than about 50 eV [20]. On this basis, values of N_v for the rare earths in Table A.1 have been computed from the sum of the chemical valence [21] and the 6 5p electrons that contribute strongly to the energy-loss spectrum [17]; these values of N_v are larger than those recommended in Version 1.0 of the database where N_v was equated to the valence. There is now a non-physical discontinuity, however, between the N_v values for the rare earths and those for Cs, Ba, and La. Further work is needed to establish the influence of 5p-electron excitations in the latter three elements and of similar core-electron excitations for other elements in groups IA, II, and III of the Periodic Table [17].

For compounds, N_v is calculated from the sum of contributions from each constituent element (i.e., N_v for each element multiplied by the chemical or estimated stoichiometric coefficient for that element).

Values of the bandgap energy E_g for many compounds can be found in a number of books [22-26]. Table A.2 contains values of E_g for some elements and representative compounds. If a value for the bandgap energy E_g cannot be found for the compound of interest, it is satisfactory to estimate this parameter because the IMFP is not a sensitive function of E_g [15,27]. For highly ionic compounds such as the alkali halides, E_g is generally between 6 eV and 11 eV. For oxides, E_g is often between 1 eV and 9 eV.

Table A.1. Recommended values for the number of valence electrons per atom (the parameter N_v) for each element for which IMFPs can be computed in the database.

Z	Element	N_v
1	H	1
2	He	2
3	Li	1
4	Be	2
5	B	3
6	C	4
7	N	5
8	O	6
9	F	7
10	Ne	8
11	Na	1
12	Mg	2
13	Al	3
14	Si	4

15	P	5
16	S	6
17	Cl	7
18	Ar	8
19	K	1
20	Ca	2
21	Sc	3
22	Ti	4
23	V	5
24	Cr	6
25	Mn	7
26	Fe	8
27	Co	9
28	Ni	10
29	Cu	11
30	Zn	12
31	Ga	3
32	Ge	4
33	As	5
34	Se	6
35	Br	7
36	Kr	8
37	Rb	1
38	Sr	2
39	Y	3
40	Zr	4
41	Nb	5
42	Mo	6
44	Ru	8
45	Rh	9
46	Pd	10
47	Ag	11
48	Cd	12
49	In	3
50	Sn	4
51	Sb	5
52	Te	6
53	I	7
54	Xe	8
55	Cs	1
56	Ba	2
57	La	3
58	Ce	9
59	Pr	9
60	Nd	9
62	Sm	9

63	Eu	8
64	Gd	9
65	Tb	9
66	Dy	9
67	Ho	9
68	Er	9
69	Tm	9
70	Yb	8
71	Lu	9
72	Hf	4
73	Ta	5
74	W	6
75	Re	7
76	Os	8
77	Ir	9
78	Pt	10
79	Au	11
80	Hg	12
81	Tl	3
82	Pb	4
83	Bi	5
90	Th	4
91	Pa	3
92	U	3

Table A.2. Values of the band gap energy E_g for elements and selected compounds (at room temperature) from the indicated references.

Material	E_g (eV)	Reference
B	1.55	24
C (diamond)	5.4	24
Ge	0.67	24
Se (gray)	1.5	24
Si	1.107	24
Sn (alpha phase)	0.08	24
Te	0.33	24
AgBr	2.50	24
AgCl	3.0	20
AgI	2.63	24
AlAs	2.16	24
AlN	6.02	24
AlP	2.5	20

AlSb	1.60	24
BN	4.6	24
CdS	2.42	24
CdSe	1.74	24
CdTe	1.5	24
Cu ₂ O	2.2	20
GaAs	1.35	24
GaN	3.34	24
GaP	2.24	24
GaSb	0.67	24
HgTe	0.2	20
InAs	0.36	24
InN	2.0	24
InP	1.27	24
InSb	0.16	24
KCl	8.5	20
MgO	7.3	20
NaCl	8.6	20
PbS	0.5	24
PbSe	0.37	24
PbTe	0.25	24
SiC (alpha phase)	2.86	24
TiO ₂ (rutile)	3.05	20
ZnO	3.2	24
ZnS	3.6	24
ZnSb	0.56	20
ZnSe	2.58	24
ZnTe	2.26	24

G-1 Equation of Gries

Gries [7] developed the following equation for the prediction of the IMFP λ (in Ångstroms):

$$\lambda = 10k_1(V_a / Z^*)E/(\log E - k_2) \quad (\text{A.7})$$

where $V_a = M/\rho$ is the atomic volume (in cm³ mol⁻¹), Z^* is a parameter found empirically to be equal to $Z^{1/2}$, Z is the atomic number (for an element), and k_1 and k_2 are parameters. Values of k_1 and k_2 were found from fits of Eq. (A.7) to the IMFPs calculated by Tanuma *et al.* [5,6,15] for groups of selected elements and compounds: 0.0020 and 1.30 for the 3d elements (Ti-Cu); 0.0019 and 1.35 for the 4d elements (Zr-Ag); 0.0019 and 1.45 for the 5d elements (Hf-Au); 0.0014 and 1.10 for the remaining elements (with which Y is included instead of the 4d elements; 0.0018 and 1.00 for organic compounds; and 0.0019 and 1.30 for inorganic compounds. The terms V_a and Z^* in Eq. (A.7) were generalized by Gries to apply to a compound $A_pB_q, \dots C_r$, with corresponding atomic numbers $Z_A, Z_B, \dots Z_C$ and atomic weights $M_A, M_B, \dots M_C$, as follows:

$$Z^* = (pZ_A^{1/2} + qZ_B^{1/2} + \dots + Z_C^{1/2}) / (p + q + \dots + r) \quad (\text{A.8})$$

$$V_a = (pM_A + qM_B + \dots + rM_C) / \rho(p + q + \dots + r) \quad (\text{A.9})$$

Equations (A.7) through (A.9) constitute the G-1 equation.

Atomic Weight and Density Data

Numerical data for atomic weights and material densities are needed for evaluation of the TPP-2M equation of Tanuma *et al.* and the G-1 equation of Gries.

The database makes use of atomic weights recommended by the International Union of Pure and Applied Chemistry in 1995 [28]. Elemental densities have been obtained from Ref. 29 and are shown in Table A.3. Other Handbooks containing density data were reviewed and numerous (generally small) discrepancies were found. Since the conditions of measurement in the various sources were not specified (and no references were provided), it was not possible to make a selection of data on scientific criteria. Instead, densities from Ref. 29 have been arbitrarily assumed to be “correct.” If more reliable density data becomes available for particular elements, suitable adjustments can be made to IMFPs or EALs obtained from the database using the equations given above. The calculated IMFPs of Tanuma *et al.* for carbon in the database are for glassy carbon with a density of 1.8 g cm⁻³ [6]; IMFPs can be calculated in the database with the Gries G-1 equation [Eqs. (A.7-A.9)] using either the density for graphite or for diamond in Table A.3. Densities for inorganic compounds and organic compounds can be obtained from Refs. 29 and 30, respectively.

Tanuma *et al.* developed an earlier predictive IMFP formula, designated TPP-2, based on calculated IMFPs for a group of 27 elements [6]; this predictive equation was later modified, in one parameter, to become the TPP-2M equation given above after consideration of calculated IMFPs for a group of 14 organic compounds [5]. The extent to which an IMFP calculated from the TPP-2 equation depends on material density has been analyzed for several representative elements and inorganic compounds [6,27]. Similar tests have not been made for the TPP-2M equation although it is thought that the earlier tests with the TPP-2 equation should provide general guidance. The database can, of course, be utilized to examine the variation of calculated IMFPs for a material of interest with different assumed densities in the TPP-2M and G-1 equations.

Table A.3. Densities of elemental solids at or near room temperature [29].

Z	Element	Density (g cm ⁻³)
3	Li	0.534
4	Be	1.85
5	B	2.34
6	C	2.2 (graphite) 3.513 (diamond)
11	Na	0.97
12	Mg	1.74
13	Al	2.70
14	Si	2.3290
15	P	1.823 (white) 2.16 (red) 2.69 (black)
16	S	2.07
19	K	0.89
20	Ca	1.54
21	Sc	2.99
22	Ti	4.506
23	V	6.0
24	Cr	7.15
25	Mn	7.3
26	Fe	7.87
27	Co	8.90
28	Ni	8.86
29	Cu	8.96
30	Zn	7.14
31	Ga	5.91
32	Ge	5.3234
33	As	5.75
34	Se	4.39 (alpha phase) 4.28 (vitreous phase) 4.81 (gray)
37	Rb	1.53
38	Sr	2.64
39	Y	4.47
40	Zr	6.52
41	Nb	8.57
42	Mo	10.2
44	Ru	12.1
45	Rh	12.4
46	Pd	12.0

47	Ag	10.5
48	Cd	8.69
49	In	7.31
50	Sn	5.769 (gray) 7.265 (white)
51	Sb	6.68
52	Te	6.24
55	Cs	1.93
56	Ba	3.62
57	La	6.15
58	Ce	6.770
59	Pr	6.77
60	Nd	7.01
62	Sm	7.52
63	Eu	5.24
64	Gd	7.90
65	Tb	8.23
66	Dy	8.55
67	Ho	8.80
68	Er	9.07
69	Tm	9.32
70	Yb	6.90
71	Lu	9.84
72	Hf	13.3
73	Ta	16.4
74	W	19.3
75	Re	20.8
76	Os	22.59
77	Ir	22.5
78	Pt	21.5
79	Au	19.3
80	Hg	13.5336
81	Tl	11.8
82	Pb	11.3
83	Bi	9.79
90	Th	11.7
91	Pa	15.4
92	U	19.1

Appendix B

EXAMPLE OF A FILE CONTAINING INELASTIC MEAN FREE PATHS

The listing shown below is an example of an IMFP data file produced by the database. This file was created using the Inorganic Compounds option of the Database option on the main menu, the option to calculate IMFPs from predictive formulae, the TPP-2M equation of Tanuma *et al.* [5], and parameters for silicon nitride.

COMPOUND: SILICON NITRIDE

SOURCE:

 Tanuma, Powell & Penn
 Surface Interface Anal. 21 (1994) 165
 Values of IMFP obtained from TPP-2M equation

MOLECULAR WEIGHT: 140.28346

DENSITY: 3.4400 g/cm**3

TABULATION:

Energy eV	IMFP Angstroms
50.000	5.83
100.000	6.26
150.000	7.10
200.000	8.10
250.000	9.13
300.000	10.17
350.000	11.19
400.000	12.21
450.000	13.22
500.000	14.21
550.000	15.19
600.000	16.16
650.000	17.12
700.000	18.07
750.000	19.01
800.000	19.94
850.000	20.86
900.000	21.78
950.000	22.69

1000.000	23.59
1050.000	24.49
1100.000	25.37
1150.000	26.26
1200.000	27.14
1250.000	28.01
1300.000	28.88
1350.000	29.74
1400.000	30.60
1450.000	31.46
1500.000	32.31
1550.000	33.15
1600.000	34.00
1650.000	34.84
1700.000	35.67
1750.000	36.50
1800.000	37.33
1850.000	38.16
1900.000	38.98
1950.000	39.80
2000.000	40.62

Appendix C CONTACTS

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

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