CHAPTER TWO

Installation and Running of the CAESAR package

2.1 Installation

The user may obtain the *CAESAR* package in a CD by contacting the authors at *info@PrimeC.com.* However, it is more convenient to download the *CAESAR* package from the web site, *www.PrimerC.com*, where the setup files are stored in the *CAESAR.ZIP* file. After downloading this file, the user should first unzip it. If the *WinZip* is installed in Windows 95 and

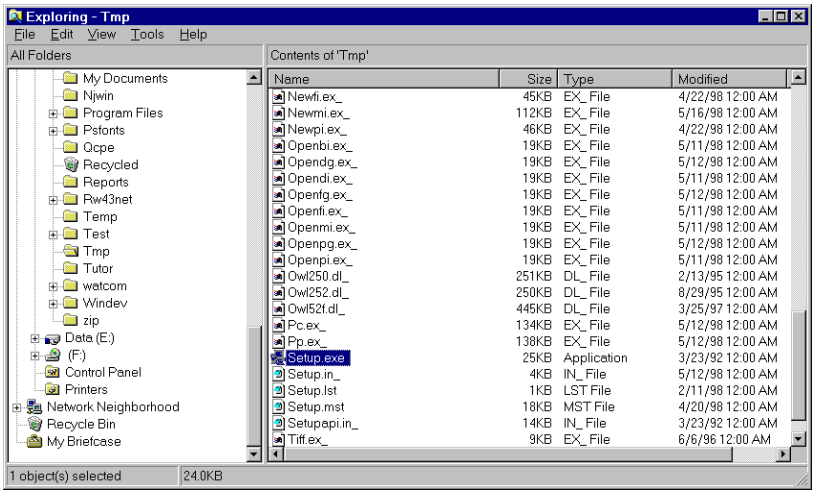

Figure 2.1. Directory containing the setup files of *CAESAR* downloaded from the network.

Windows NT, then the unzipping is achieved simply by clicking the file name *CAESAR.ZIP* from the *Windows Exploring* list. Alternatively, the *CAESAR.ZIP* file can be unzipped by using any unzip utility program (e.g., *pkunzip*). The following example makes use of the *pkunzip* program:

(1) Click the *MS-DOS Command Prompt* logo in the Windows 95 or Windows NT's *Start* popup menu. Then the user will be in the system drive, which is drive C in most cases.
(2) Switch to the disk drive and directory where the *CAESAR.ZIP* file resides, and use the command "*pkunzip CAESAR.ZIP*".

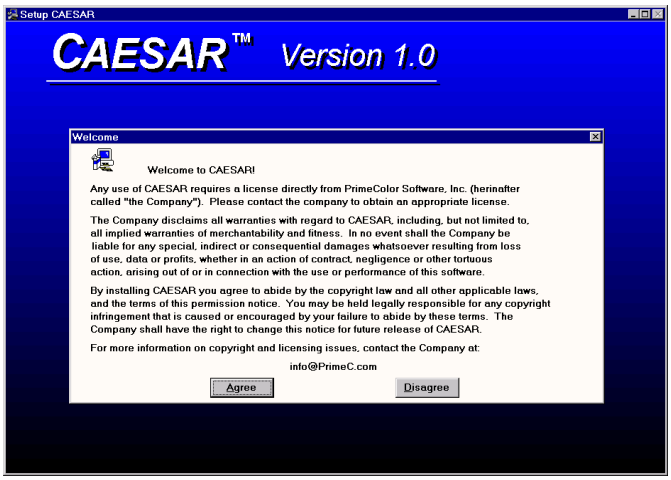

Figure 2.2. Setup CAESAR window.

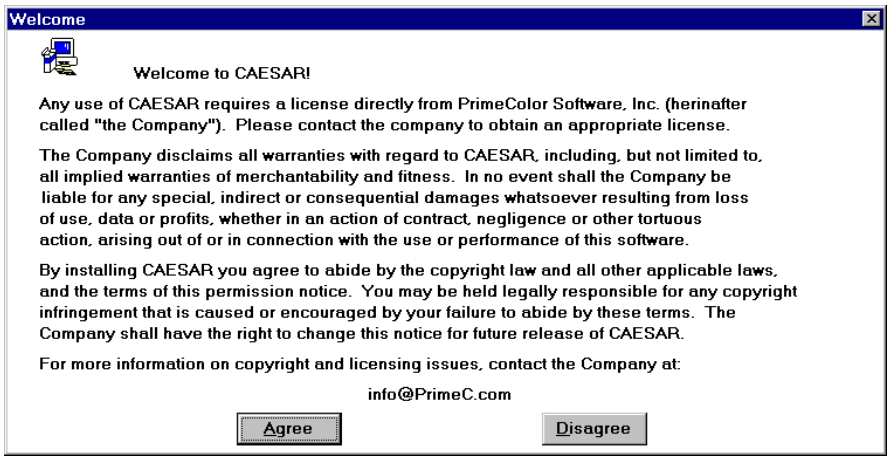

Figure 2.3. Welcome dialog box.

To install the *CAESAR* package using the setup CD, click the CD drive icon in the *Windows Exploring* list. If the *CAESAR* package was downloaded from the web site, click the icon of the directory containing the setup files in the *Windows Exploring* list (*Figure 2.1*). Then, click the file *Setup.exe* to open the *Setup CAESAR* window (*Figure 2.2*). This window shows the copyright and licensing statements in the *Welcome* dialog box (*Figure 2.3*) and two buttons, *Agree* and *Disagree*. If the user cannot accept the conditions described in the *Welcome* box, click the *Disagree* button to open the *Quit Setup* dialog box and confirm the exit operation (*Figure 2.4*). The *Exit* button opens the *Early Exit Message* dialog box (*Figure 2.5*), which will interrupt the setup procedure and close the *Setup*

CAESAR window. When the *Exit* button is selected at any stage of the installation, the *Quit Setup* and the *Early Exit Message* dialog boxes open to terminate the setup procedure. If the *Continue* button of the *Quit Setup* dialog box is selected, the box disappears and the control is returned to the previous dialog box.

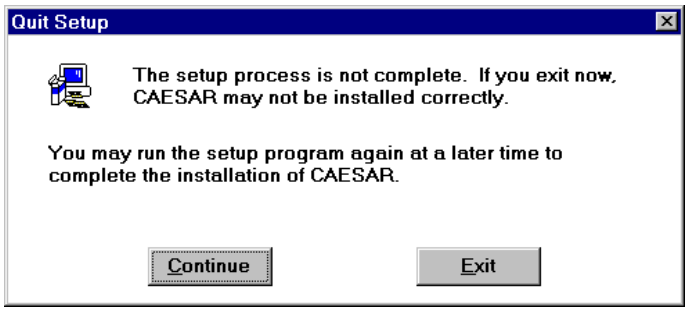

Figure 2.4. Quit Setup dialog box.

Figure 2.5. Early Exit Message dialog box.

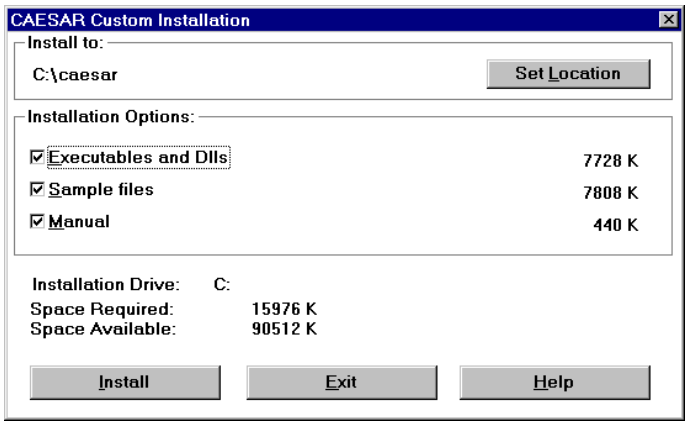

Figure 2.6. CAESAR Custom Installation dialog box.

If the conditions stated in the *Welcome* box are acceptable, click the *Agree* button to continue the setup procedure. This opens the *CAESAR Custom Installation* dialog box (*Figure 2.6*). The *Install to:* field is used to define the disk drive and the destination directory in which to store the *CAESAR* package. By default, the disk drive C: and the CAESAR directory are used. To run the application

programs of the *CAESAR* package, it is necessary obtain the license file *CAESAR.AUT* from the authors of the *CAESAR* package by contacting them at *info@PrimeC.com*. The authors create the license file using the serial number of the disk drive of a user's PC in which to install the *CARSAR* package. The serial number of any disk drive of a PC can be found by following the steps given below.

(1) Click the *MS-DOS Command Prompt* logo in the Windows 95 or Windows NT's *Start* popup menu. Then the user will be in the system drive, which is drive C in most cases.

(2) If this is the drive in which to install the *CAESAR*, enter the command "VOL". Then the needed information appears as shown in the following example:

Volume in drive C is NTSystem.
Volume Serial Number is 5884-3C54.

(3) If the user wants to install the package in a different drive, e.g., drive D, then change the current directory to drive D by entering the command "D:" and then use the command "VOL" to find the volume serial number of drive D.

It is crucial to install the package in the disk drive whose serial number was used to obtain the license file, *CAESAR.AUT*. If the disk drive C: is not the drive in which to install the CAESAR, click the *Set Location* button to open the *Destination Path for CAESAR* dialog box (*Figure 2.7*). After specifying the *Path* field, click the *Continue* button to save the setting and return to the *CAESAR Custom Installation* box. The *Back* button will keep the default setting and return the control to the *CAESAR Custom Installation* box. The *Exit* button will terminate the setup procedure.

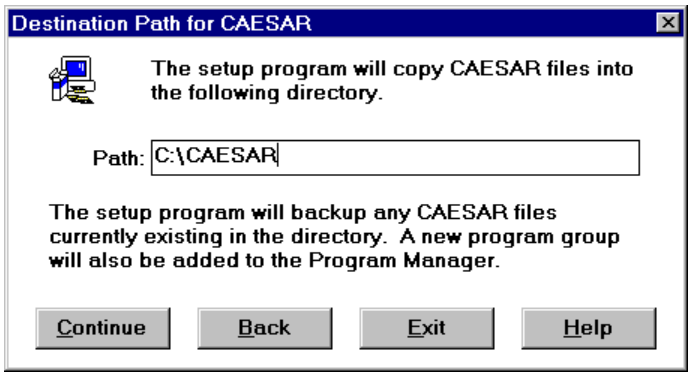

Figure 2.7. Destination Path for CAESAR dialog box.

Figure 2.8. Warning message for insufficient disk space.

The *Installation Options:* of the *CAESAR Custom Installation* box is used to select the files to be copied into the destination directory. This box shows the size of the executable modules, sample files and documents. If the available space is insufficient for backing up all desired files, a warning message will appear (*Figure 2.8*). If there is enough space in the destination drive, a dialog box will

show the backup process (*Figure 2.9*). The setup procedure will terminate normally after showing the *Exit Message* (*Figure 2.10*).

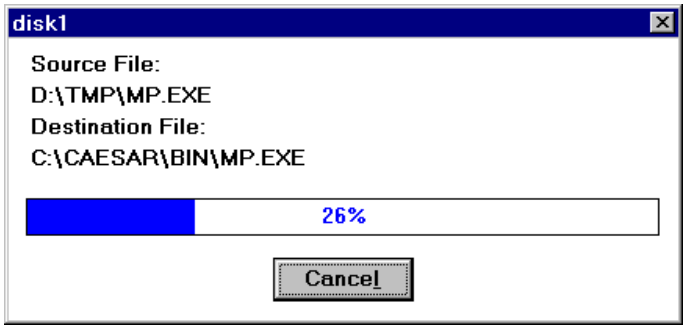

Figure 2.9. Dialog box for the backing up process.

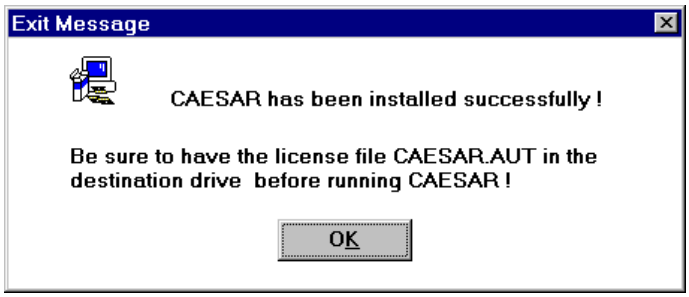

Figure 2.10. *Exit Message* dialog box.

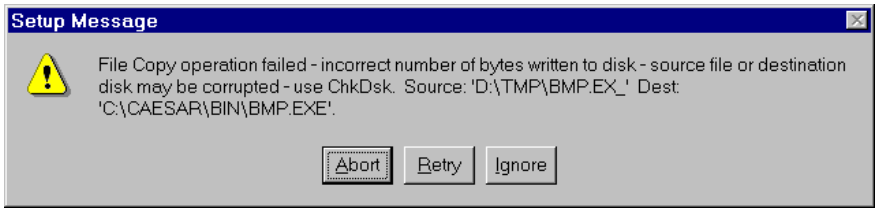

Figure 2.11. *Setup Message* dialog box.

Figure 2.12. *Setup Message* for exit.

If there are internal damages in the setup files, then the *Setup Message* box appears (*Figure 2.11*). When errors are not fatal, the user can continue the installation by clicking the *Ignore* or *Retry* button. Otherwise, click the *Abort* button to open another *Setup Message* box (*Figure 2.12*) and confirm the exit operation. The *Yes* button terminates the setup procedure after showing the *Error Message* box (*Figure 2.13*).

Figure 2.13. *Error Message* dialog box.

A successful installation automatically creates the *CAESAR* group box (*Figure 2.14*). All the executable application files are listed in the *Windows 95's Start* list under the group name *Caesar*.

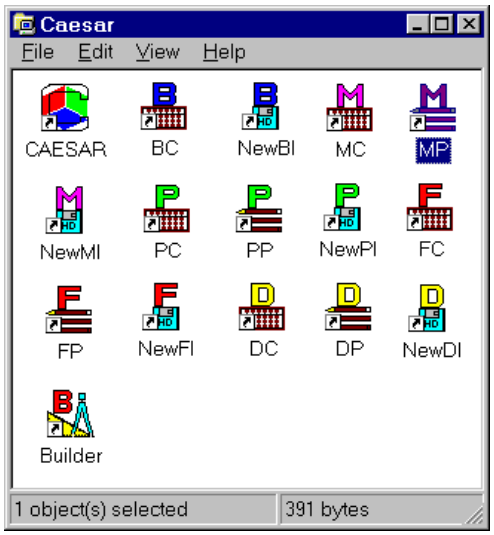

Figure 2.14. Program group *CAESAR*.

2.2 Licensing

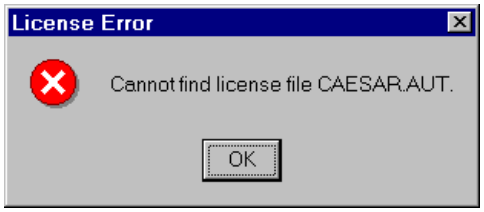

Figure 2.15. Warning dialog box for no license file.

To use the *CAESAR* package, one should purchase the license file, *CAESAR.AUT*. For details of how to obtain this file, see the web page of *www.PrimerC.com*. The license file *CAESAR.AUT* is created based on the serial number of the disk drive of the user's PC in which to install the *CAESAR* package. The user should copy the *CAESAR.AUT* file to the CAESAR directory of the disk drive where all the executable and DLL files of the *CAESAR* package reside. Failure to setup the license file correctly will cause the warning box to appear on the screen (*Figure 2.15*) and will prevent the *CAESAR* package from functioning.

2.3 Running the programs of *CAESAR*

The *CAESAR* package is written for PC's with Windows 95 and Windows NT operating systems and their updates. Once installed properly, the programs of the *CAESAR* package will reside in the CAESAR\BIN directory. To run the programs of this package, the user should go to the CAESAR\BIN directory where all the programs of the *CAESAR* are stored. By clicking the BIN icon, the user can see the contents of the CAESAR\BIN directory on the *Exploring-BIN* window (*Figure 2.16*).

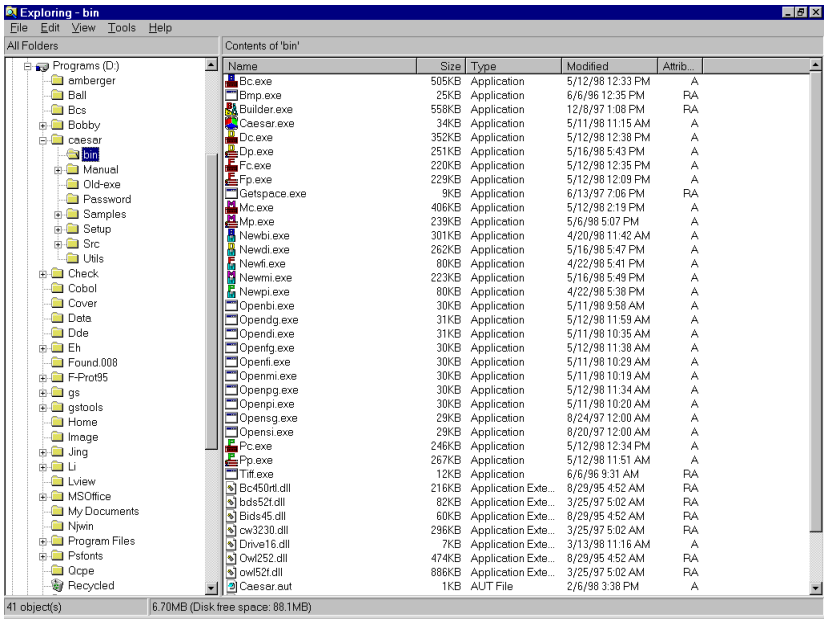

Figure 2.16. Exploring - bin window.

In general, the running of the *CAESAR* package involves (1) making inputs interactively, (2) calculating with prepared inputs, and (3) analyzing and displaying results of calculations interactively. Each program of *CAESAR* can be run separately by double clicking its icon in the BIN directory. However, it is much more convenient to launch these programs by using the popup menu on the logo page of *CAESAR* (*Figure 2.17*; see *Section 2.4*).

2.3.1 Analysis of crystal structure

The *Builder* program requires an input file, *filename.CI*. When a required input file exists, one should open it by using the *Open* command of the *File* menu in the *Builder* window. Then the structure corresponding to the input file appears on the *Builder* window. From here on, the user can analyze and manipulate the structure by using other menus of the *Builder* window.

If a required input file does not exist, the user should select the *New* command of the *File* menu in the *Builder* window. This opens the *Define Crystal Structure* window, which lets the user construct

a crystal structure file, *filename.CI*, interactively by specifying the space group information, the unit cell parameters and the fractional coordinates of the unique atoms of a unit cell. On leaving the *Define Crystal Structure* window, the crystal structure defined by the user appears on the *Builder* window. At this point, it is recommended to save the structure as a *filename.CI* file in a proper file directory.

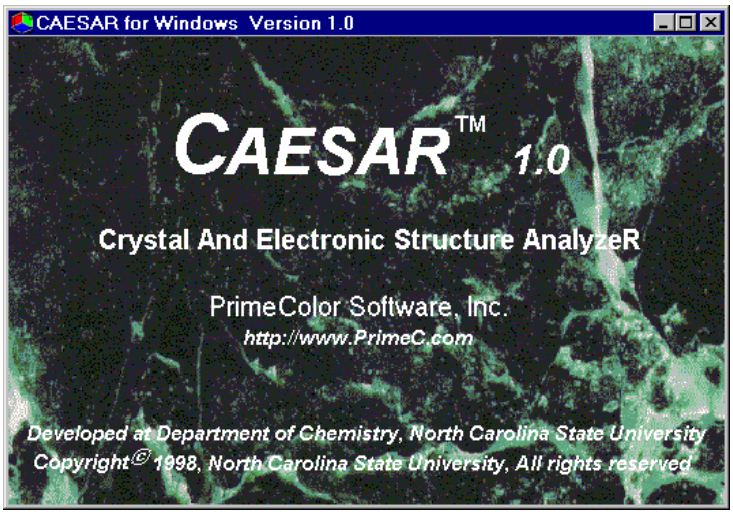

Figure 2.17. Logo window *CAESAR for Windows Version 1.0*.

The user can modify an existing *filename.CI* file to generate a new *filename.CI* file. For this purpose, the user should first open the existing file in the *Builder* window and then select the *Modify Crystal...* command of the *Build* menu in this window. Then, the *Define Crystal Structure* window opens with all the contents of the existing *filename.CI* file copied into the appropriate fields of the *Define Crystal Structure* dialog box. The user can peruse these data and modify them when necessary to produce a modified *filename.CI* file.

2.3.2 Analysis of molecular electronic structure

MO calculations for a molecule are carried out by running the program *MC*. This program requires an input file, *filename.MI*. When a required input file exists, double-click the *MC* icon. Then the *MC* window appears, which is followed by the *Open* window. The latter allows the user to open a needed input file. Once this file is opened, the *Confirmation* box appears to ask whether the user selected a correct input file. The *Yes* button makes the *MC* program run.

If a required input file, *filename.MI*, does not exist, it should be generated by running the *NEWMI* program, which opens the *New .MI File* window. This window lets the user construct a necessary input file, *filename.MI*, interactively. After completing the construction of a *filename.MI* file, it should be saved in a proper directory.

The *Modify* button of the *New .MI File* window permits the user to modify an existing *filename.MI* file to generate a new *filename.MI* file. When this button is double-clicked, the contents of the existing *filename.MI* file are copied into the appropriate fields of the *New .MI File* dialog box. The user can peruse these data and modify them when necessary to produce a modified *filename.MI* file.

The outputs of running the *MC* program serve as the inputs for the *MP* program. Thus the *MP* program can be run only after running the *MC* program.

2.3.3 Analysis of crystal electronic structure

Electronic band structure calculations for a solid are carried out by running the program *BC* as a function of wave vector for a set of wave vector points selected by the user. This program requires an input file, *filename.BI*. When the *BC* program is launched, the *BC* window appears, and then the *Open* window follows. The latter allows the user to open an existing input file. Once this file is opened, the *Confirmation* box appears to ask whether the user selected a correct input file. The *Yes* button makes the *BC* program run.

If a required input file, *filename.BI*, does not exist, it should be generated by running the *NEWBI* program, which opens the *New .BI File* window. This window lets the user construct a necessary input file, *filename.BI*, interactively.

The *Modify* button of the *New .BI File* window permits the user to modify an existing *filename.BI* file to generate a new *filename.BI* file. When this button is double-clicked, the contents of the existing *filename.BI* file are copied into the appropriate fields of the *New .BI File* dialog box. The user can peruse these data and modify them when necessary to produce a modified *filename.BI* file.

To analyze the results of running the *BC* program, it is necessary to run the program *PC*. This program requires an input file, *filename.PI*. When the *PC* program is launched, the *PC* window appears, and then the *Open* window follows. The latter allows the user to open a needed input file. Once this file is opened, the *Confirmation* box appears to ask whether the user selected a correct input file. The *Yes* button makes the *PC* program run.

If a required input file, *filename.PI*, does not exist, it should be generated by running the *NEWPI* program. When the icon of *NEWPI* is double-clicked, the *New .PI File* window opens. This window lets the user construct a necessary input file, *filename.PI*, interactively.

The *Modify* button of the *New .PI File* window permits the user to modify an existing *filename.PI* file to generate a new *filename.PI* file. When this button is double-clicked, the contents of the existing *filename.PI* file are copied into the appropriate fields of the *New .PI File* dialog box. Then the user can peruse these data and modify them when necessary to produce a modified *filename.PI* file.

The outputs of running the *PC* program serve as the inputs for the *PP* program. Thus the *PP* program can be run only after running the *PC* program, which in turn can be run only after running the *BC* program.

2.3.4 Analysis of Fermi surface

When a solid under examination is a normal metal, it may be necessary to examine its Fermi surfaces. To carry out this analysis, the user must first run the *BC* program using the *DOS/Fermi surface* option as the *Calculation Option* in the input *filename.BI* (see the *New .BI File* window of the *NEWBI* program) and then run the *FC* program.

The *FC* program requires an input file, *filename.FI*. When the *FC* program is launched, the *FC* window appears and then the *Open* window follows. The latter allows the user to open a needed input file. Once this file is opened, the *Confirmation* box appears to ask whether the user selected a correct input file. When the *Yes* button is clicked, the *FC* program starts to run.

If a required input file, *filename.FI*, does not exist, it should be generated by running the *NEWFI* program, which opens the *New .FI File* window. This window lets the user construct a necessary input file, *filename.FI*, interactively.

The *Modify* button of the *New .FI File* window permits the user to modify an existing *filename.FI* file to generate a new *filename.FI* file. When this button is double-clicked, the contents of the existing *filename.FI* file are copied into the appropriate fields of the *New .FI File* dialog box. The user can peruse these data and modify them when necessary to produce a modified *filename.FI* file.

The outputs of running the *FC* program serve as the inputs for the *FP* program. Thus the *FP* program can be run only after running the *FC* program.

2.3.5 Analysis of electron density plots

The partial and total electron density plots of a solid and a layered structure on a cross-section plane are calculated by running the *DC* program, which requires an input file, *filename.DI*. When the *DC* program is launched, the *DC* window appears, and then the *Open* window follows. The latter

allows the user to open a needed input file. Once this file is opened, the *Confirmation* box appears to ask whether the user selected a correct input file. The *Yes* button makes the *DC* program run.

If a required input file, *filename.DI*, does not exist, it should be generated by running the *NEWDI* program. When the icon of *NEWDI* is double-clicked, the *New .DI File* window opens. This window lets the user construct a necessary input file, *filename.DI*, interactively.

The *Modify* button of the *New .DI File* window permits the user to modify an existing *filename.DI* file to generate a new *filename.DI* file. When this button is double-clicked, the contents of the existing *filename.DI* file are copied into the appropriate fields of the *New .DI File* dialog box. The user can peruse these data and modify them when necessary to produce a modified *filename.DI* file.

Results of running the *DC* program serve as the input for the *DP* program. Thus the *DP* program can be run only after running the *DC* program.

2.4 Launching the programs from the *CAESAR* logo page

The window *CAESAR for Windows Version 1.0* (*Figure 2.17*) appears when the *CAESAR* logo of the CAESAR\BIN directory is clicked. This window stays as the top window on the screen unless it is closed by the user. A hand-indicator appears whenever the mouse cursor moves inside the window area. When clicked, the mouse button opens the popup menu (*Figure 2.18*), from which the user can launch any one of the 15 application programs of the *CAESAR* package. During the execution of a selected program, the *CAESAR* logo window is minimized. After completing the run, the logo window is maximized again to allow the user to choose another program to run. Thus it is more convenient to run the programs of the CAESAR package using the popup menu of the *CAESAR* logo than to launch them directly from the CAESAR\BIN directory.

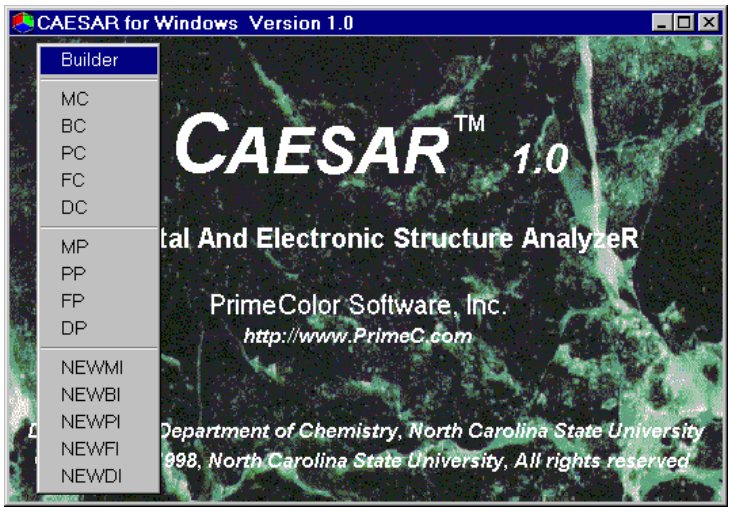

Figure 2.18. Popup menu for launching the application programs of the CAESAR package.