

LCELLS Manual

System Requirements

1. Win95/98/Me; NT4/Win2k/XP
2. Pentium 133 MHz, 64Mb memory
- 3a. PKZIP (or equivalent) is required if you need to read archive files
- 3b. PATH variable must include the folder with the PKZIP software
4. Read/write access to drive C: (folder C:\CIFS_TMP) and the program's installation folder is required

Installation

The program can be installed on the computer simply by copying the executable file CIFS.EXE.

Description

The program allows (a) the creation of a database of crystallographic files, including those in ZIP archives, located on specific computers and (b) searches for unitcells using either original (input) or Niggli reduced cell.

Interface Description

The *Main window* (Figure 1) consists of the main menu, controls to manage cell input, viewers for both the list of files found and the individual files. After you have input the cell parameters and lattice type, the *Update Cell* button will generate the reduced (Niggli) cell. If the cell search procedure finds any hits the corresponding files will appear in the list. Individual files can be examined in the file viewer simply double clicking on their names. The file currently being viewed can be saved to disk by pressing the *Save File As ...* button. If no hits are found, try increasing the value of the *deviation*: you may thereby find a cell that was determined poorly, or at a different temperature, or one that is related, for example the cell for an isostructural compound.

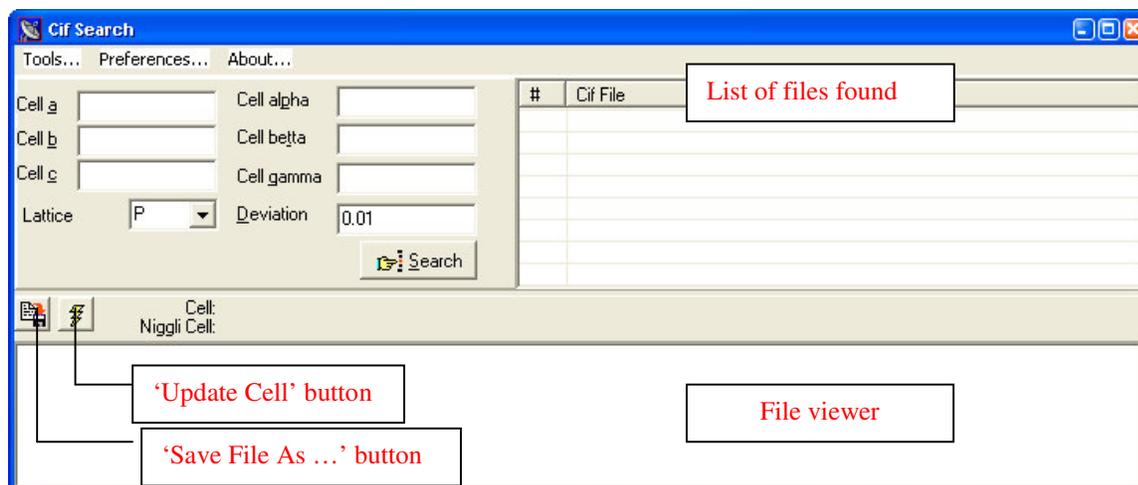


Figure 1. View of the main window

The *Tools...* menu brings up the *Index Info* window (see Fig 2a), which shows index information and various tools. There are three ways to update or create an index in this dialog:

1. *All drives* – the program searches throughout all allowed volumes, including CD and network drives.
2. *From Folder* – you need to specify the folder by pressing the ... (*ellipsis*) button.
3. *Using the List* – you need to create a list of folders using *Preferences...* menu in the main window.

You can specify the size of the largest file to be included in the search: this avoids wasting time searching large archive files that do not contain any relevant information. *Index cleanup* operations help to keep your index in a specific state: you have the option to delete *duplicate records with the same cell* and remove *dead links*. “Dead

links” are links to non-existing files, so when you use this option, be careful, as in case of absence of network connection all references to network files will be removed from index file.

The **Preferences** menu brings up a window (see Fig 2b) where you can specify (top) a list of folders from which the index should be updated and (bottom) a list of index files. Index files speed up cross-network searches because the index can be updated more quickly on the local computer.

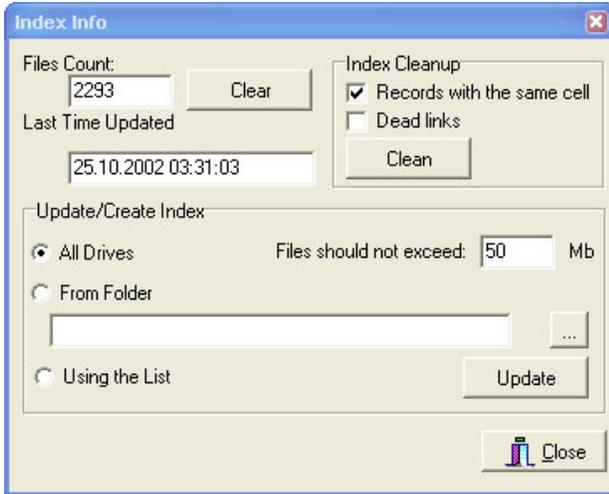


Figure 2 (a) View of **Index Info** window

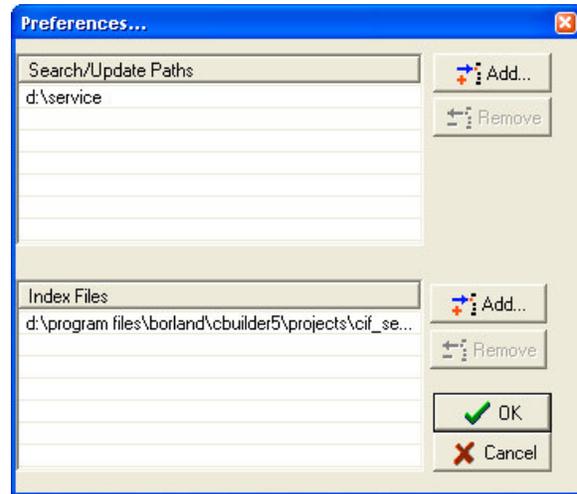


Figure 2(b) View of **Preferences** window

Automated index update

The index file can be updated automatically, using the list of folders. To do this you can schedule the program and run it with the 'update' switch.