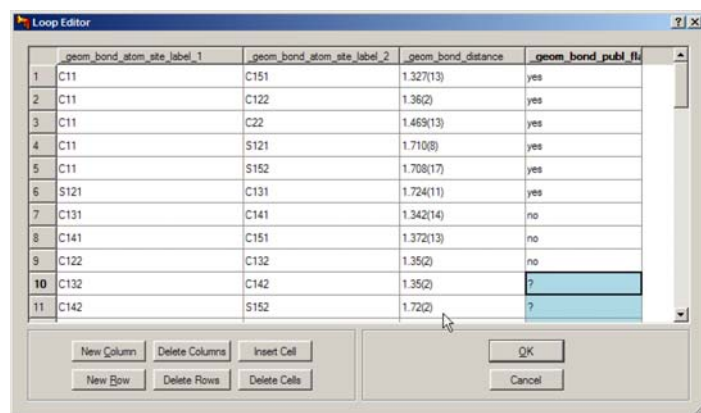


5.3. SYNTACTIC UTILITIES FOR CIF



	geom_bond_atom_ite_label_1	geom_bond_atom_ite_label_2	geom_bond_distance	geom_bond_publication
1	C11	C151	1.327(13)	yes
2	C11	C122	1.36(2)	yes
3	C11	C22	1.469(13)	yes
4	C11	S121	1.710(8)	yes
5	C11	S152	1.708(17)	yes
6	S121	C131	1.724(11)	yes
7	C131	C141	1.342(14)	no
8	C141	C151	1.372(13)	no
9	C122	C132	1.35(2)	no
10	C132	C142	1.35(2)	?
11	C142	S152	1.72(2)	?

Fig. 5.3.3.2. The *enCIFer* loop editor.

block is flagged as an error. The program log in the lower right-hand part of the program window records the history of the user's interactions with the file during the current editing session.

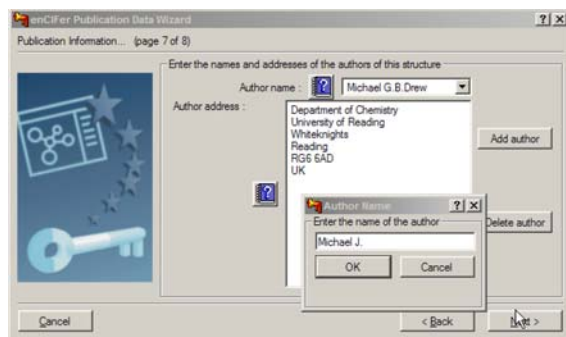
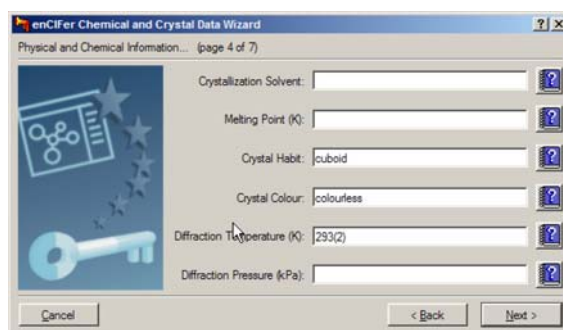
Information is written to the status bar (the lower margin of the window) to indicate the location by line and column number of the editing cursor.

5.3.3.1.7. *The loop editor*

The program has a useful spreadsheet-style editor for looped lists (Fig. 5.3.3.2). A particular benefit of this style of display is that the spreadsheet cells are arranged in a rectangular grid, so that visual scans can often detect deviations from a pattern of values within a column, thus making it easy to identify placement errors where values have been omitted or inadvertently conjoined. Such errors are not always obvious by direct visual inspection of a CIF, where the layout of a looped list need not follow any regular pattern.

The buttons to add or delete columns allow for the straightforward addition or deletion of data items from the loop. If the user selects the 'New Column' button, a small pop-up window helpfully provides a view of the associated dictionary (in the same hierarchical category-based tree view of the dictionary browser pane) to help the user select the required new data name. The 'Insert Cell' and 'Delete Cells' buttons are convenient tools for the realignment of rows and columns where values have been omitted or misplaced.

The loop editor is invoked from one of two buttons in the task bar, allowing either the creation of a new looped list or the modification of an existing one. As with the application as a whole, there is no dynamic validation of input; the new list must be saved and the entire CIF then manually revalidated.

Fig. 5.3.3.3. The *enCIFer* publication data wizard. Information about the title and authors of an article to be submitted for publication is requested through a sequence of linked dialogue boxes.Fig. 5.3.3.4. The *enCIFer* chemical and crystal data wizard.5.3.3.1.8. *The publication and chemical and crystal data wizards*

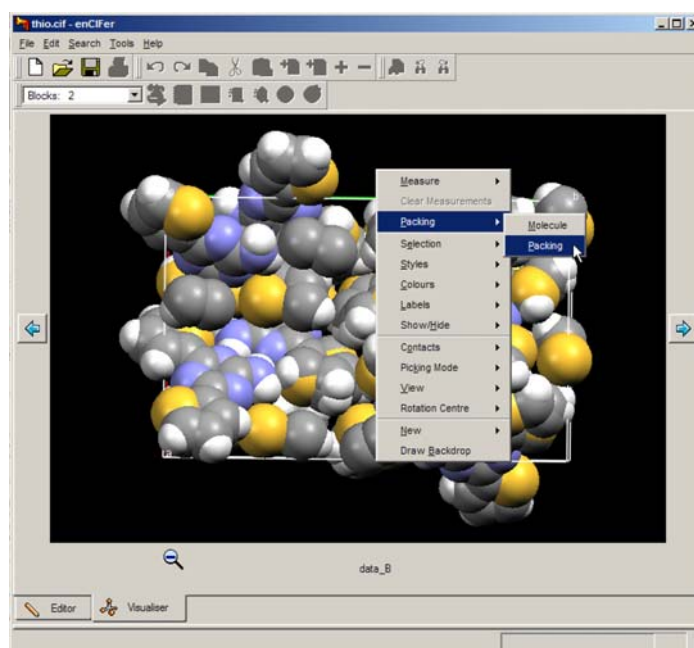
The user may invoke data-entry 'wizards', subordinate programs that prompt for particular data items useful for the publication of a crystal structure report or for the deposition of a crystal structure in a database. This is the kind of information that might be requested in the *Notes for authors* for a journal, and it is helpful if the information is routinely requested from inexperienced authors during normal use of the software. The data-entry tools are known as 'wizards' because they will utilize information already in the file.

Hence, as shown in Fig. 5.3.3.3, details of an article's contact author are retrieved from the CIF and used to seed a list of contributing authors. As the address for each author is entered, the program makes each new address available as a stored record for easier input of additional information.

Fig. 5.3.3.4 demonstrates the same approach to encouraging authors to supplement information already in the CIF with related chemical (or crystal) data not usually provided by the CIF generators embedded in crystallographic structure determination programs.

5.3.3.1.9. *The visualization window*

A final useful feature of *enCIFer* is its ability to visualize the three-dimensional structure of molecules described in the data blocks of a CIF. Fig. 5.3.3.5 demonstrates crystal packing with

Fig. 5.3.3.5. Visualization of a molecular and crystal three-dimensional structure with *enCIFer*.