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1. Description of the problem

The identification of previously encountered unit cells can save considerable amounts of diffractometer time by preventing the inadvertent and unwanted recollection of data sets on known compounds or phases. While published unit cells are searchable *via* the Cambridge Structural Database (Allen & Kennard, 1993) or the Inorganic Crystal Structure Database (Belsky *et al.*, 2002), large numbers of unpublished local cells can pose a problem. The ability to create, update and search a database of such cells can therefore increase efficiency in the structure determination laboratory.

2. Description of the program

The program has two functions: to create or update an index (database) of unit cells from existing structure files located on local or network disk volumes, and to search this index for a cell input by the investigator. Importantly, the program does not require any reformatting or re-entry of existing data.

2.1. Creating and updating the index file

Creation of the index file requires the specification of a location on a local or network drive. The program searches this location and any subdirectories for structure files: the current version looks for *SHELXL* (Sheldrick, 1997) instruction files and Crystallographic Information Files (CIF; Hall *et al.*, 1991), adding the unit-cell information they contain to the index. The program also searches for these files in archives created using the *PKZIP* program (*PKWARE*, 1993). It is possible to save time by limiting the search to relevant folders. Updating the index files is similar to creation but generally requires much less time. An index file containing 10000 unit cells is approximately 1.5 Mbyte in size.

2.2. Search engine

The required input data for a unit-cell search comprise six unit-cell parameters, the lattice type and an agreement limit (default 1%). The search proceeds by comparison of the input cell parameters, as input, following circular rotation of the parameters ($\{a–b–c, \alpha–\beta–\gamma\}$, $\{c–a–b, \gamma–\alpha–\beta\}$, $\{b–c–a, \beta–\gamma–\alpha\}$) and, for centred cells, by Niggli reduction (Křivý & Gruber, 1976). Searching an index of 10000 unit cells takes less than 2 s on a PC with a 1.5 GHz Pentium processor.

3. Software environment

LCELLS runs under Windows 98/ME/NT4/2000/XP. The user interface and main program are written in Borland C++.

4. Documentation and availability

A two-page manual in PDF format contains system requirements, installation notes and a description of the user interface. The program is available on request from the principal author.

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