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1. The crystallographic problem

Crystallographers need to make a number of simple algebraic calculations in order to obtain lengths, angles, define relations between molecules, transformations of the coordinates, *etc*. These calculations can be performed by general means, *e.g.* either with a pocket calculator or with a computer using standard mathematical packages. Another possibility is to have a specialized tool, tuned particularly to these calculations, easy to call and to use, and fast to address the problem.

2. Method of solution

A new program in the suite of Tcl/Tk-based programs (Urzhumtseva & Urzhumtsev, 1996, 1997, 1998, 1999), named *CALCRYS*, has been developed. This program allows one to work with vectors defined either in real or in reciprocal three-dimensional space, expressed either in Cartesian or in crystallographic (fractional) coordinates. Unit cells can be defined also either in real or in reciprocal space. When the cell is defined, its parameters in the conjugate space and all metrical tensors can be calculated automatically. The optional choice of the orthogonalization agreement allows the orthogonalization and deorthogonalization matrices to be established automatically. This crystallographic information is presented permanently on screen (Fig. 1).

The available algebraic operations include the calculation of a linear combination of vectors, their scalar and vector product (taking into account the corresponding metrical tensors), the product of a matrix with a vector or another matrix, a linear combination of matrices, matrix inversion, matrix determinant, *etc*. These operations are gathered in a menu displayed near the set of work windows containing the data with which these operations are executed. Another field contains a number of 'memory cells' which allow intermediate results to be saved (any mixture of numbers, vectors or matrices) and used later. Information can be inserted into the working windows in several ways: copied from the crystallographic field, from the memory cells, directly typed or read from a file.

Some other crystallographic packages (see *e.g.* Siegrist, 1997) can in particular make similar calculations. The main difference between such programs and *CALCRYS* is that the latter addresses a more specific problem and as a consequence is much simpler: it does not use any script and all its operations are realised through the menu; it runs on any computer, does not need any installation procedure and is distributed freely.

3. Software and hardware environment

The program *CALCRYS* is written in Tcl/Tk (Ousterhaut, 1993). It can be run under Unix on an SGI computer, on a DEC Alpha station, or on an IBM PC under Windows, with the Tcl/Tk libraries installed. The program can be also run on a Macintosh with an X-terminal emulator, *e.g. Exodus*.

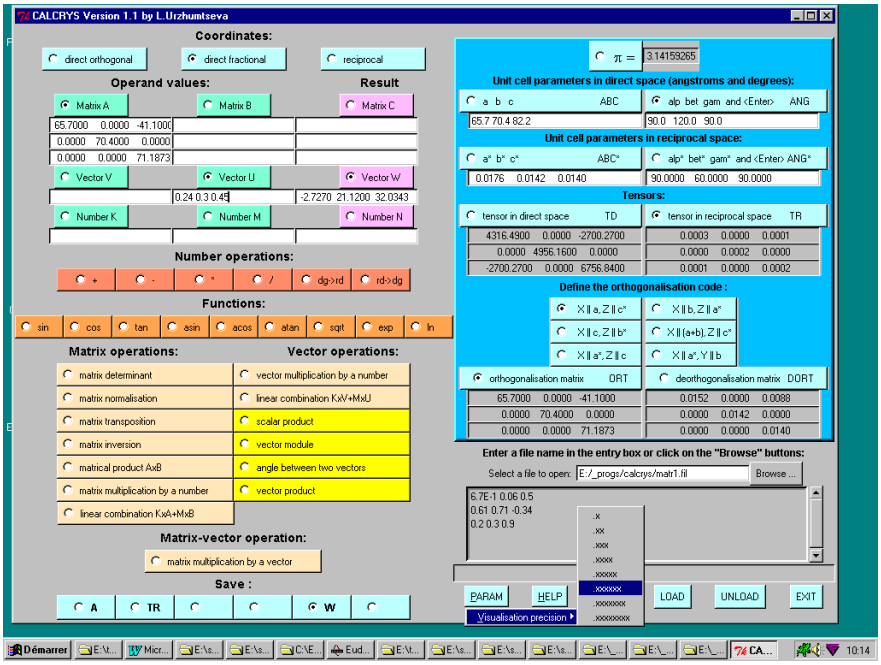

Figure 1
Screenshot of the program form.

4. Documentation

No special documentation is necessary, owing to the menu-based character of the program.

5. Availability

The program can be used by researchers as well as by students and teachers of crystallography. It is available from the authors upon request.

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