Symmetry and crystallography: New facilities in the graphic software MANOSK

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The new routine SYMCRY of the graphics program MANOSK is described in this paper. It is designed to analyze interactions between molecular structures related by crystalline symmetry. The symetric objects can be described in the same referential, to be manipulated as an entity, or in a referential of their own, to undergo correlative real-time movements (via the dials), given the symmetry constraints. Crystal packing can be observed, and any command of the main software MANOSK is available for the symmetric objects, including storage of the coordinates of symmetrics in the final orientation.

Keywords: symmetry, crystallography, computer graphics

INTRODUCTION

More and more interactive graphic softwares allow the three-dimensional exploration of biological, organic and inorganic compounds. However, very few allow manipulation of crystal structures and more precisely of molecular (sub)structures linked by symmetry elements. The first programs to allow the representation of crystal packing, ORTEP,[1] and PLUTO,[2] generated two-dimensional plots, and the stereoimages gave quite a good idea of what the structure might be.

More recently, the softwares CHEM-X,[3] and PLUVA,[4] and also MANOSK,[5] running on E&S PS300 graphic systems, have offered the possibility of visualizing and manipulating interactively a crystal packing, but without providing all the facilities for complete analysis. In this paper, we will describe the new option SYMCRY of the graphics package MANOSK, which allows the display, manipulation, and complete analysis of symmetry-related objects.

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INPUT

As shown in Figure 1, the option SYMCRY can be achieved after loading and displaying the "unique atoms," i.e., the asymmetric unit. The type of coordinates file must be ASCII, and different standard formats are available: PDB,[6] Protin,[7] CSSR.[3] Cartesian coordinates in Angströms or fractional coordinates are initially accepted, and the routine SYMCRY converts the cartesian coordinates into fractional ones, after checking the unit cell parameters.

The symmetry operations relative to the space group concerned can be introduced via the keyboard or via a data file, in the syntax used for the description of the complete Wyckoff positions in the International Tables.[8] A set of files describing the most common space groups is available. During execution, it is possible to add symmetric structures, by giving interactively the new symmetry operations; cell translations can also be added to any translation defined by any symmetry operation. For a better understanding of intermolecular contacts, automatic translation of the objects in the cell can be selected. The translatory operations are worked out for the geometric center of each symmetric and are stored in specific tables; the symmetric structures are instantaneously translated in the cell, which can be screened by picking the item "CELL" in the menu. Finally, the total translation on each symmetric is the translation defined by the space group, plus the cell translation that has been added.

DISPLAY AND MANIPULATION

The symmetric structures can be handled via the dials in two different ways, respectively by the options FIXSYM and MOVSYM. In the option FIXSYM, the rotations de-

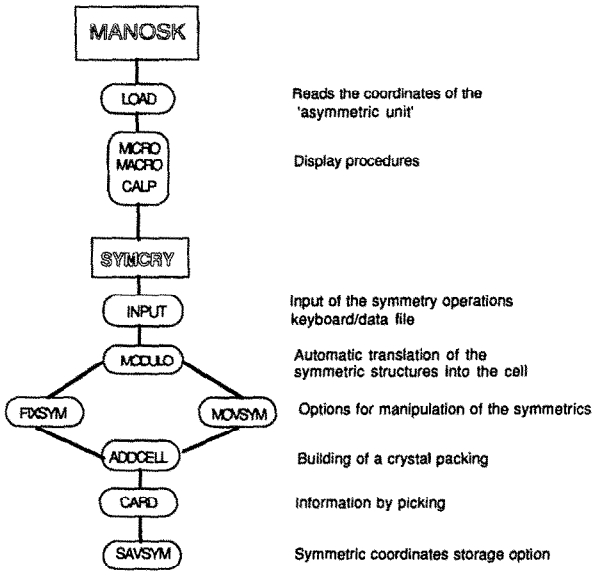

Figure 1. Organization of the option SYMCRY in the main graphic software MANOSK

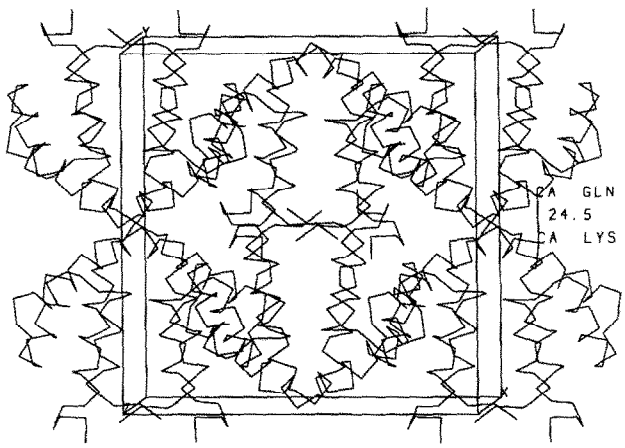

Figure 2. Display of the eight symmetry-equivalent structures of Uteroglobin,[9] -space-group $C222_1$- using the options FIXSYM and MODULO. An illustrative calculation of an intersymmetric distance between the structures represented by their carbon alpha chains is shown

fined by the symmetry operations and the total translations are applied to the "asymmetric unit." Each symmetric generated is characterized by its own graphic object in such a way that any information can be achieved by picking, as exemplified in Figure 2. All structures are fixed models, taken together as an entity; they undergo the same movements when the user turns the dials. In MOVSYM, the symmetrics have their own referential, and their movements through the dials are interdependent. In this case, all the symmetric structures belong to the main graphic object called "molecule," which also contains the objects describing the "asymmetric unit" (molecular surface,[10] van der Waals surface, spline,[11] labels, bonds, etc.). The shifts of the asymmetric unit are echoed in real time on all the symmetry-

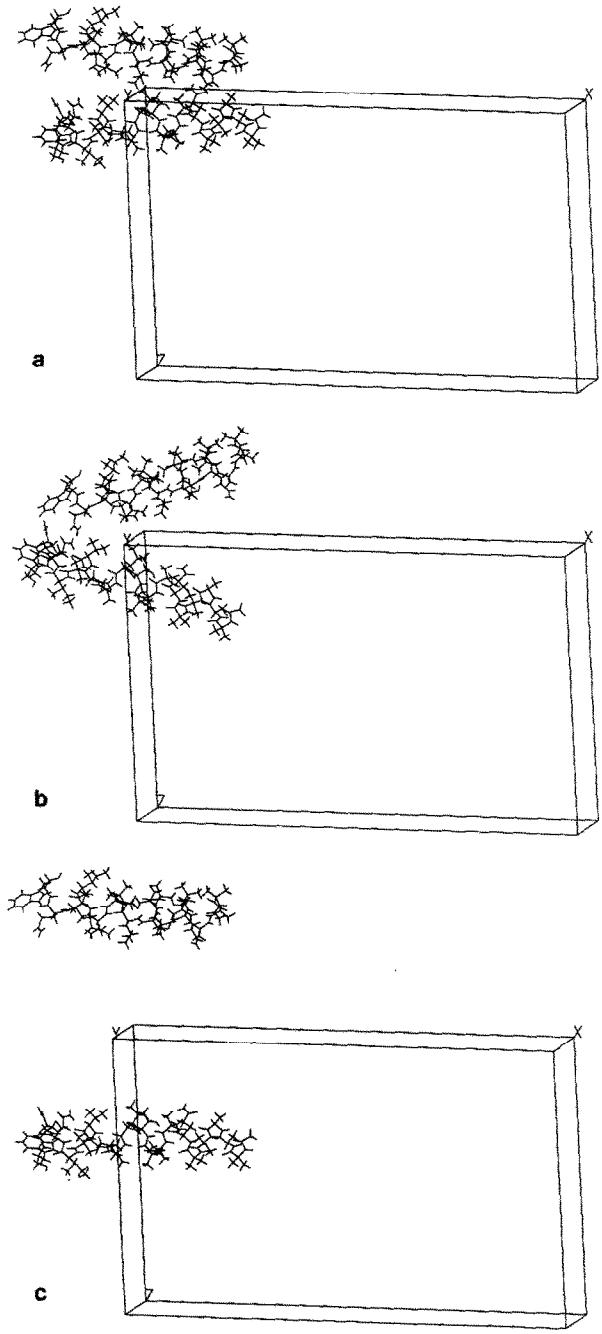

Figure 3. (a) Representation of the asymmetric unit of Trichorzianin A1 (above) and of the symmetry-equivalent molecules generated by the operation X,–Y,–Z (below), in their initial positions; (b) A rotation around the Y *axis is inversely echoed on the molecules; (c) The same symmetry-related objects after a translation on the* Z *axis. They have undergone opposite translations towards this axis*

related objects, with regard to the crystal symmetry of the space group. This new way of displaying symmetrics is done without redefining each atom of the symmetrics, that cannot be identified by picking, but using the PS300 graphic function network. This feature allows a really fast display of symmetrics and of physical properties of every symmetric. Figure 3 illustrates this option with two symmetry-

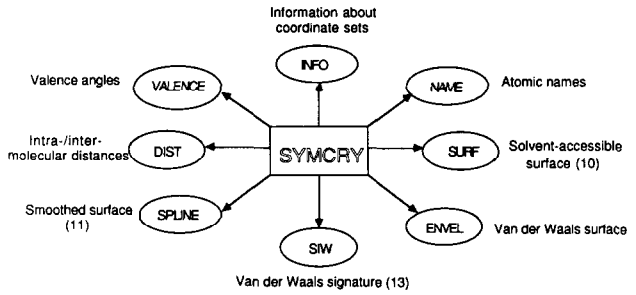

Figure 4. Interactions between the module SYMCRY and the other modules in MANOSK

equivalent molecules of Trichorzianin A1,[12] generated respectively by the symmetry operations X,Y,Z and X,–Y,–Z.

The user can study consecutively the structures with two options, without redefining the symmetry operations. Picking the items "SYM" and "MVSY" allows screening of the symmetrics generated respectively by FIXSYM and MOVSYM.

ANALYSIS AND OUTPUT

The usual facilities of the main program MANOSK are available for this module as shown in Figure 4: information on the labels of the atoms of the symmetrics, calculation of interatomic distances between the symmetrics, calculation of valence angles, etc. The calculation and display of molecular surface, van der Waals surface, and van der Waals signature[13] (*cf.* Color Plate 1) are also available from the SYM options. By picking any atom of the symmetrics, the option CARD provides information on the name of the atom, its symmetric number, and the symmetry card and the symmetry operations used to generate it. The user can assign a color either to symmetric structure or to each amino acid.

Automatic crystal packing can be computed with the option ADDCELL, which allows the building of a parallelepiped of 8 or 27 initial cells, or of N initial cells in the M direction, with N and M to be interactively specified by the user. The visualization of such packings, as exemplified in Color Plate 2, provides a perfect idea of the environment of one cell, and this is especially interesting for the analysis of layered structures.

After the analysis, the coordinates of the structures of the symmetrics in their final orientation can be stored in a file, either in cartesian or fractional coordinates, and in any format offered by the input process. After the option FIXSYM, the coordinates of each symmetric are written out, whereas after the process MOVSYM, only the coordinates of the asymmetric unit can be stored. In this latter case, the set of symmetry-equivalent objects can be generated by using the option FIXSYM again. It is possible to store in an output file the symmetry operations and total translations worked out on each symmetric structure.

SUMMARY

The molecular modeling software MANOSK has now enlarged its facilities to the field of crystallography, by the new routine SYMCRY, which allows the visualization, manipulation and analysis of symmetry-linked structures. For example, it can be helpful for molecular replacement, since it allows easy handling of crystal packing and access to any information on any symmetric. The possibility of manipulating symmetric objects with retention—or not—of the crystalline symmetry, provides a good method for molecular refinement studies.

The MANOSK package is available for academics and industries through an ANVAR licence on request to Dr. J. P. Mornon.

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