# Program for the visualization and interactive study of molecules on a calligraphic display system

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*Mops is a computer program for the visualization and interactive analysis of crystallographic and molecular structures on a calligraphic PS 300 display system. This system allows the interactive display of bond lengths, bond angles and torsion angles with colour coding of atom types as well as crystalline packing interactions. Mops is also capable of easily drawing a chosen image on the screen using the Ortep program. This facility allows the very fast preparation of slides or illustrations.*

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The examination and analysis of 3D structures, molecules and their assemblies (as found for example in crystal packings or in molecular complexes), require the ability of representing them either on static 2 or 3D graphics or, more efficiently, dynamically on raster and vector graphic systems. Whatever the method used to determine these structures (X-ray crystallography or molecular modelling coupled with energy refinement), there has always been an important need for powerful, easy to handle tools, in order to help their visualization not only by crystallographers and chemists but more recently by immunologists and biologists. For a long time, programs such as Ortep[1] and Pluto[2], have been considered as standard for both mono and stereoscopic bidimensional viewing of molecules. These programs require trial-and-error procedures to find the optimum orientation of the molecule, or the help of an automatic program to compute the rotation around a suitable weighted molecular inertia system to minimize overlaps and preferentially show given atoms[3].

Because the cost of interactive graphic stations has fallen in recent years, they are now available in more and more laboratories (linked to minicomputers), and have enabled great progress in molecular modelling using both raster or calligraphic viewing devices[4]. This has increased the demand in the field of interactive graphic softwares. Recently, the introduction of a standalone calligraphic system allowing real-time object manipulation and viewing, gave a new impetus in the field of molecular graphics. Apart from programs such as Frodo[5], Bilder[6] and Sybil which were immediately adapted to be used with these systems, there was a need for programs providing greater versatility and easier handling of molecular viewing. Such programs would allow the rapid preparation of slides or molecular drawings.

Mops was designed to visualize any molecule or part of molecule obtained from a databank or determined by structural analysis; using Mops it is possible to represent thermal motion ellipsoids, a facility which previously was only feasible with Ortep[1]. The program provides a direct and very efficient way of preparing drawings by allowing a fast choice of the desired orientation of the model. It has been written to provide all the features that help in the examination of a molecule, such as real-time manipulation, editing facilities to prepare pictures for publication or teaching, as well as the possibility to obtain information about distances, bond angles and torsional angles. The advantages of such a program, almost independent from the host computer, is its ease of use, the small demand on host computer time and the efficient visualization of an object which can then be drawn as a 2D picture.

## IMPLEMENTATION

Mops is implemented on an Evans & Sutherland PS 300 calligraphic system running under the A.1 operating system. This is connected to either a 16-bit DEC PDP 11/44 or a 32-bit DEC VAX 11/750 computer running respectively under RSX11M V4.1 and VMS V4.2 installed in the Institut de Biologie Moleculaire et Cellulaire du CNRS, Strasbourg (France). The programs are written in FORTRAN 77 and PS300 programming languages. A standard RS 232 communication line at 9600 baud is used to link the computers and the graphic display system.

## OVERVIEW OF THE MOPS PACKAGE

Mops is based on two independent programs: Psmol, written in FORTRAN 77 prepares all the data to be sent to the graphics system in order to 'build' the desired object; Mops, operating within the graphic display, deals with the representation and editing of the model on the screen, allowing full interactive manipulation of the

observed molecules or assembly of atoms written in PS300 language:

### Psmol: a program to handle general information

The primary role of Psmol is to handle the preparation of the list of atomic positions of the object to be displayed. Coordinates can be derived from an atom data file as defined in the SDP package[7] or also from any formatted atom files such as the Cambridge Structural Database[8].

When information is obtained through the SDP data files (STRUC.NME and PARA.DTE) the program can directly use all the information contained in them. This includes:

- space group and cell parameters,
- names of the atoms for identification and assignment of conventional colours,
- fractional atomic coordinates and thermal motion parameters for the display of crystallographic structure,
- symmetry operations generating a full object from the asymmetric unit and generating symmetry related atomic positions.

In the absence of the SDP files, an interactive dialogue asks for all the necessary information and stores them in new data files. The STRUC.NME file contains the general structural information and the PARA.DTE file contains the general atomic parameters.

After selection of the atoms, the program allows either fully automatic construction of the bonds between atoms by using a dictionary of standard bond length, or an interactive construction through a dialogue where each bond is specified. A colour specification is requested for each type of atoms to be displayed. As has already been stated, symmetry operations are dealt with during this process to generate a full object. Symmetry related atomic positions can be optionally indicated in order to show, for example, molecular packing. The only limits in the number of atoms that can be displayed is the number of vectors displayed on the graphics system simultaneously.

### Mops: a program to handle 3D molecular models

Mops has several main functions: interactive display, structure analysis facilities and preparation of graphics or slides. These activities, described later in the text, can be activated either from the keyboard or with the dials from the graphic station. A detailed description of the menu is shown in Tables 1 and 2.

Colour Plate 1 shows an example of a molecule of (2*S*,*SS*)-methionine-sulphoximine[9] drawn on the graphic system with Mops. Atoms are colour coded; the model depth cued can be represented as both a mono or true stereoscopic image. This compound and its molecular packing are also represented as stereoscopic views in Colour Plates 2 and Colour Plates 3, respectively. Real time rotation, translation, clipping and scaling (orthogonal or perspective) are available.

Editing facilities can be activated directly from the keyboard of the PS300. They include bond creation or breaking. Groups of atoms in different classes can be switched on and off; this leaves the backbone of the molecule intact. The backbone can also be switched on and off independently. If crystallographically equivalent molecules are desired to be drawn, the original model can be displayed alone but with its equivalents.

Standard structure analysis facilities are available. They include atom identification and specification of atomic distances, angles and torsional angles. Atoms displayed on the screen can be picked using a data tablet. All functions, clearly identified by light emitting diodes, can easily be selected using the PS300 keyboard.

When connected to an host computer, the graphic system provides the orientation matrix to be used in Ortep[1] to obtain the drawing of the actual image on the screen (see Colour Plates 1–3). This interactive facility allows the very fast preparation of illustrations.

**Table 1. Description of the command keys available on the Evans & Sutherland PS300**

| Keys | Initial | Activation | Function |
|---|---|---|---|
| 1 | – | – | Not used |
| 2 | – | – | Not used |
| 3 | ORIENT | ORIENT | Orientation matrix is sent to the host computer |
| 4 | NO-BOND | NO-BOND | No action |
| | | NEW-BOND | A new bond is created between two picked atoms (with Key 5 : PIC-ATOM) |
| 5 | PIC-ATOM | PIC-ATOM | Atoms are 'pickable' |
| | | PIC-BOND | Breaks the 'picked' bond |
| 6 | Representation of the original model | | |
| | MOLE=ORG | MOLE=ORG | Backbone and atoms of the original model |
| | | MOLE=EQV | Original model has the same representation that the equivalents (with Key 8) |
| 7 | Several sets of atoms can be displayed (with Key 6 : MOLE=EQV and Key 8 : EQV: ....) | | |
| | NO-ATOM | NO-ATOM | No atoms |
| | | ATOMS 1 | Only atoms of type 1 |
| | | ATOMS 2 | Only atoms of type 2 |
| | | ... | ... |
| | | ATOMS | All atoms |
| 8 | Several representations of the equivalents are available (with Key 6 : MOLE=EQV) | | |
| | NO-EQV | NO-EQV | No equivalent |
| | | EQV:BOND | Backbone only |
| | | EQV:ALL | Backbone and atoms |
| | | EQV:ATOM | Atoms only (with Key 7) |
| | | EQV:DOTS | Dots instead of atoms |
| 9 | NO-CLIP | NO-CLIP | Clipping is set on and off |
| 10 | MONO | MONO | Mono, stereo, left or |
| | | STEREO | right view of the model |
| | | LEFT | |
| | | RIGHT | |
| 11 | DIALWIND | DIALWIND | The dials 5, 6 and 7 are switched |
| | | DIAl-FOV | (See Table 2) |
| | | DIALTRAN | |
| 12 | ORTHOG | ORTHOG | Orthogonal projection |
| | | PERSPE | Perspective projection |

## CONCLUSION

The Mops program described in this paper has been developed in order to facilitate the dynamic representation of molecular structures obtained from databanks. Using Mops, the investigator can quickly obtain Ortep

**Table 2. Description of the command dials available on the Evans & Sutherland PS300**

| Dials | Initial | Activation | Function |
|---|---|---|---|
| 1 | ROTX | ROTX | Rotation around the horizontal axis of the screen |
| 2 | ROTY | ROTY | Rotation around the vertical axis of the screen |
| 3 | ROTZ | ROTZ | Rotation around the perpendicular axis of the screen |
| 4 | SCALE | SCALE | Scale factor applied to the image |
| 5 | W-FRONT | W-FRONT | Positioning of the front plane in orthogonal projection (with Key 11: DIALWIND) |
| | | F-FRONT | Positioning of the front plane in perspective projection (with Key 11: DIAL-FOV) |
| | | TRANX | Translation along the horizontal axis of the screen (with Key 11: DIALTRAN) |
| 6 | W-BACK | W-BACK | Positioning of the back plane in orthogonal projection (with Key 11: DIALWIND) |
| | | F-BACK | Positioning of the back plane in perspective projection (with Key 11: DIAL-FOV) |
| | | TRANY | Translation along the vertical axis of the screen (with Key 11: DIALTRAN) |
| 7 | TRANZ | TRANZ | Translation along the axis perpendicular to the screen (with Key 11: DIALWIND or DIALTRAN) |
| | | ZOOM | Zooming angle of perspective projection (with Key 11: DIAL-FOV and Key 12: PERSPE) |
| 8 | STEREO | STEREO | Separation of the left and right stereoscopic views (with Key 10: STEREO) |

drawings and colour slides of structures. Molecules displayed using Mops have bond lengths, bond angles and torsion angles colour coded for easy interpretation. The program is easy to handle. All documentation and help functions (as well as an installation procedure) are available on request — in tape form.

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