Computer graphic tool for colour structure display on personal computers

P Cozzini, P Pavesi and G D Andreetti

Istituto di Strutturistica Chimica, Università di Parma, Via M D'Azeglio 85, 43100 Parma, Italy

The aim of the work was to implement a package to produce a colour molecular display on a low-cost personal computer. The package provides colour representation of a structure like a single molecule or molecules in a cell. Using this package, the researcher (chemist, pharmacist or biologist) can show a compound, or a class of compounds, whose structure has been solved by X-ray or neutron diffraction. The work demonstrates that it is possible to have a stand-alone colour graphic workstation with a low investment.

Keywords: graphics, personal computer, chemistry

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During the last ten years a number of graphic systems have been developed for researchers to model and study molecular structures; nevertheless these packages run mainly on a mainframe or on a minicomputer and require a colour workstation. The high cost of these solutions prevents the researcher from using the various capabilities of these packages.

The problem was to develop a colour graphic workstation, easily used by a chemist, producing molecular displays with different features (display, rotation, zoom, clipping, plotting, etc.). The package Pluto, of Cambridge crystallographic files, which runs batch on a CDC 7600 and Ortep and produces monochromatic graph plots was available in the University computing centre.

An interactive version similar to Pluto named CSD, Crystal Structures Display, running on CDC 6600 and using a monochromatic Tektronix series 4010 or 4050 was available. The package named Video-mol has been created on a 16-bit personal computer.

METHOD AND HARDWARE

The problem was to show a three-dimensional system on the bidimensional plane of a video screen to give the best quality of pictures. The technique of the clinographic projection was adopted as it seemed to be quite a good system, well known to chemists and already widely used. The matrix to be applied to the atomic coordinates is

$-\sin(18°\ 26')$	$\cos(18°26')$	0
$-\cos(18°26')\ tg12$	$-\sin(18°\ 26')\ tg12$	1
1	0	0

for the clinographic axes of Figure 1.

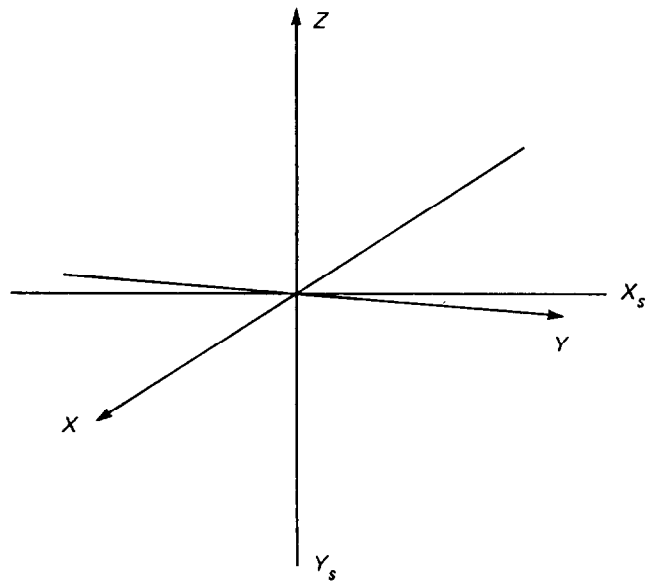

Figure 1. Clinographic axes; $X_s = -X\sin(18°\ 26'), +Y\cos(18°\ 26'), Y_s = -X\cos(18°\ 26')\ tg12° - Y\sin(18°\ 26')\ tg12° + Z$

The following hardware was available:

- a personal computer Zenith model Z-100 running with Microsoft DOS operating system release 1.0; an operating that is now standard in most personal computers: also called PC DOS (PC = IBM);
- a minicomputer Gould-Sel: Cambridge Crystallographic Data Bank files are available through the Centro di Studio per la Strutturistica Diffrattometrica del CNR.

SYSTEM CONFIGURATION

Personal computer Zenith Z-100

Hardware:

- CPU 16 bit 8086;
- CPU 8 bit 8085;
- 128 kbyte RAM;
- 2 floppy disk drives 5″ 1/4 (320 × 2 kbyte capacity);
- standard graphic adapter;
- standard colour graphic monitor medium resolution (640 × 225 pixels);
- graphic tablet Houston Hi-pad connected to the serial port; and
- dot-matrix serial printer Centronics 704.

 0263-7855/85/030090-03$03.00

Software:

Operating system: ZDOS-Zenith implementation of MSDOS release 1.0;

Language: ZBASIC-Zenith version of Microsoft BASIC with colour graphic capabilities; and

Colour: the colour graphic features depend on the hardware: different personal computers have different screen resolution and a different number and type of colours. For example: PC IBM — 320 × 200 pixels × 16 colours; 600 × 200 B and white; and PC Olivetti and PC AT & T — 600 × 400 B and white × 16 grey levels; 300 × 200 × 16 colours.

The minimum requirement for the stand-alone colour graphic workstation is:

- 64 (128) kbyte RAM:
- 2 floppy disc 320 or 360 kbyte capacity (this capacity depends on the MS-DOS Operating System version);
- RGB colour monitor;
- serial tablet or a light pen;
- matrix printer;
- 1 serial port; and
- 1 parallel port (optional).

Minicomputer Gould-Sel Systems 37/77 of Centro di Studio per la Strutturistica Diffrattometrica, CNR Figure 2).

DATA DESCRIPTION AND FORMAT

The input of data is possible in two ways: either personal data input from keyboard; or series of compounds from data banks on different networks. The data of the compound that one would show on the screen can be introduced by keyboard or from local or international networks by connecting the personal computer to receive the data on floppy (or Winchester) disc.

The input data file for Videomol follows the rules of the Cambridge Crystallographic Files as this format is the standard in structural study literature. The format data is:

- Compound number, reference code, number of atoms, number of fragments;
- 4 decoding parameters;
- cell parameters;
- symmetry matrices;
- covalent radii;
- order number of fragments of atoms; and
- cordinates: atom name, coord (x), coord (y), coord (z).

The standard description of data now extends up to large weights in structural studies; this is in fact the best system to manage an exchange or a comparison of input data on a personal computer.

PACKAGE

The work session is entirely interactive and the user chooses the pathway of the work in a tree menu. The instruments which control the communication to the PC are a keyboard, a graphic tablet and a light pen. The PC uses a colour screen, a printer or a graphic colour plotter. The high resolution of the screen (640 × 225 pixels) gives a good three-dimensional colour representation.

The package consists of 30 programs which permit the use of several other available functions:

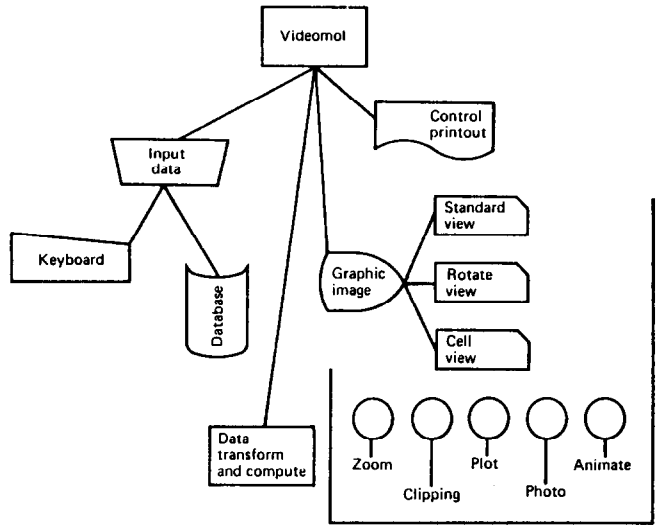

Figure 2. Logical function pathway of package

- input data;
- data transform (compute, translate format, etc.);
- display (screen and plotter); and
- control printout.

During the execution of the programs the data moves from file to file maintaining the same standard format. The structure can now be displayed in the form: standard view, that is the result of input data display; and rotate view, along x, y or z axes or along the line between two atoms (linked or not linked). The same type of display can be used for cell display.

There are three fundamental styles of drawing: solid models and conic bonds; stick models; and van der Waals radii (applied both to the entire structure or to a fragment of the structure). The ball colours follow the standard international rules of chemical compounds' representation.

During the display session control of the work can shift from the keyboard to the graphic tablet (or the light pen). In this mode the user can apply the zoom function, clipping function and other commands to the draw on the screen. It is possible to copy the drawing from the screen on a colour plotter (on a chart or a slide) and to obtain a control printout of the geometrical data on a matrix printer.

Other two important features are: copy of the screen display on colour transparency or on colour photography by photo-camera; and tape recording of scientific films, showing the structure animation on three-dimensional space. This recording can be realized by TV camera or by direct connection computer-video tape. The film production is important as it gives a complete 3D understanding of the structure (see for example Colour Plates 1–4).

The computing time, from the input data to the first display depends on the number of atoms; the total time is about 30 min for a structure with 60 atoms. The actual computing time is a few minutes. The package is now available only for the Zenith mod. Z-122 personal computer with colour expansion and the MS DOS version 1.0 operating system.

The package is being modified to run on the IBM PC or PC compatible with graphic (monochromatic or colour) expansion; the problem being the low resolution of the screen as the IBM PC does not have the same resolution as the Zenith PC.

	Zenith Z-122	IBM PC monochrome option	IBM PC Pixel mode colour	Olivetti (AT & T) M24–M21 monochrome option	Olivetti (AT & T) M24–M21 colour
No. of pixels	640 × 225	640 × 200	320 × 200	640 × 400	320 × 200
No. of col. or grey levels	8	1	4	16	4
Cost of the workstation	~$4500	~$3500	~$4000	~$3500	~$4000

The package costs US $100 and is available from the Institute of Structural Chemistry, University of Parma.

CONCLUSIONS AND FUTURE DEVELOPMENT

In this work it has been demonstrated that it is possible to have a colour graphic station for molecular display with a low investment without needing a mainframe computer. The increasing use of computer techniques in all scientific disciplines and particularly in chemistry, biology and biochemistry means that most researchers have to acquire a knowledge of new instruments. The wide availability of personal and desk-top computers makes it easy for the researcher to acquire that knowledge.

The new development will be in order to make a Multidisciplinary Informative System: a user-oriented interactive symbolic language integrated with database networks.

The aim of the project is to make a new contribution in the field of CACHE (Computer Aided Chemistry) technologies.

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