Program for the visualization of inorganic crystals

A. Dietrich and B. Maigret

Laboratoire de RMN et Modélisation Moléculaire, Institut de Chimie, Strasbourg, France

A program has been developed to manipulate images of inorganic structures and organic molecules on ALLIANT VFX/40 using the PHIGS + standard. This article reviews algorithms for representing spheres, ellipsoids and various polyhedrons involved in inorganic chemistry. The program also supports the display and manipulation of animated frames from dynamics simulations. Many graphical facilities have been implemented and we discuss their interest in the field of molecular graphics.

Keywords: 3D raster graphics, polyhedral approximation, coordination chemistry, ORTEP drawings, CPK modeling, dynamics

INTRODUCTION

High performance interactive computer graphics now make molecular structure visualization an irreplaceable process. It is becoming increasingly important in all fields of chemistry: Fast examination of three-dimensional models of molecules allows the chemist to be more efficient and creative. Several molecular visualization packages have, therefore, been developed on the most recent graphic workstations and are now available.[1-6] Except for FRODO[1] most are devoted to molecules in the gas phase or in solution and little has been done for crystal manipulation and visualization; recently some attempts have been made to fill this deficiency.[4-9]

In fact programs written several years ago provided high quality crystal drawings on plotters. ORTEP[10] is still the most popular one for crystal structure illustrations, yet it is the most difficult to handle. PLUTO[11] follows similar principles and is more convenient but is limited to ball-and-stick representation. Only STRUPLO[12] draws crystal structures in polyhedral representation, which is the most desirable representation for displaying inorganic structures.

In the present work, a general molecular graphic package has been developed on an ALLIANT[13] high performance graphic workstation. This program handles all the useful molecular representations: wire-frame and space-filing CPK, thermal ellipsoids, polyhedron and smooth molecular surfaces. It also allows animation to focus on interesting events during molecular simulation.

IMPLEMENTATION

The ALLIANT FX/40® minisupercomputer was primarily dedicated to fast job calculation but since 1988 it integrates graphics capabilities, namely two 1280 × 1024 × 24 image memory units and one 1280 × 1024 × 16 Z-buffer. The interaction devices[14] are the keyboard, the locator (a mouse), picks and buttons that are simulated by the locator, and valuators, which are physical dials or else can be simulated by the locator. Four graphics arithmetic processors (GAP)[15] perform the calculations involved in graphics output operations. They process graphic commands in parallel. The application is written in C[16] and uses the ANSI PHIGS+[17] library subroutines.

PROGRAM DESCRIPTION

We now describe what we can consider to be an interactive graphic mask. The screen (Color Plate 1) is divided into four parts of unequal size:

- The upper left part displays the molecule. This window can be magnified and saved in a file. The other three are control windows for the molecule's appearance.
- The lower left window is a side view of the scene; it displays the box extent, and the front/back clipping and depth-cueing planes. This gives appropriate feedback to the user.
- Buttons, check boxes and two static menus lie upper right. Buttons indicate whether shading, depth-cueing and perspective projections are enabled or disabled. Each check box activates a light source, which can be ambient, directional, point or spot. The first static menu is user defined. Each selection of the other static menu redefines dial box functions, including:
  - Rotation, translation, scaling and projection reference point
  - Front/back depth-cueing planes, background RGB components, front clipping plane and gap with the back one
  - RGB components of ambient light source

- RGB components of directional light and light source direction
- RGB components of point light and light source position
- Spotlight source position, direction and spread angle
- Translucency coefficient, surface properties coefficients for ambient, diffuse and specular light
- A crude drawing of the dial box fills the lower right window. Each dial is represented by a circle with its current value within and label below. This window is updated when dial functions are redefined.

ALGORITHMS

The interactive mask being settled, it is now time to draw the molecule. We first introduce three algorithms describing the basic objects involved in molecular representation.

Sphere

The icosahedron is one of the five convex and regular polyhedrons. It has 12 vertices, all of which lie on the surface of a sphere (Color Plate 2). There are 30 edges and 20 faces, which are equilateral triangles. The 12 vertices happen to lie at the corners of three golden rectangles that are symmetrically intertwined.[18] A golden rectangle has a height-to-width ratio of $1/\tau$, where τ is the *divina proportione* (also known as the golden ratio): $(1 + \sqrt{5})/2$. As each rectangle is centered about the origin, the circumscribed sphere radius r is determined by the coordinates of any one vertex. Vertex coordinates are $(0, \pm L, \pm l)$, $(\pm l, 0, \pm L)$, $(\pm L, \pm l, 0)$ with $l = r/\sqrt{(1 + \tau^2)}$ and $L = \tau \times l$. We compute vertices for the unit sphere only.

We then approximate the sphere surface by subdividing each equilateral triangle into four new ones. Let M_{01}, M_{12} and M_{20} be the midpoints of sides S_0S_1, S_1S_2 and S_2S_0, respectively. (See Figure 1). We project those points on to the sphere surface by normalizing the OM_i vectors. We join projected points, thus creating four equilateral triangles (S_0, M_{01}, M_{20}), (S_2, M_{20}, M_{12}), (S_1, M_{12}, M_{01}) and (M_{01}, M_{12}, M_{20}). We can iterate this process with new triangles. We count vertices, edges and faces as function of subdivision number n.

Number of 5-degree vertices $v_{5,n} = 12$

$v_{6,n} = 10 \times (4^n - 1)$

$e_n = 30 \times 4^n$

$f_{3,n} = 20 \times 4^n$

We can apply Euler's relation, which holds for non-bounded and orientable surfaces:

$(v_{5,n} + v_{6,n}) - e_n + f_{3,n} = 2$

$2e_n = 3f_{3,n} = 5v_{5,n} + 6v_{6,n}$

In contrast, when using the classical meridian/parallel meshes, we count:

Number of meridians m (>1)
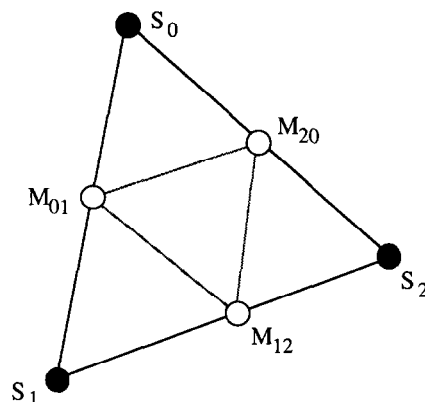
Number of parallels p (>0)

$v_{2m} = 2$

Figure 1. Equilateral triangle subdivided into four new triangles

$v_4 = 2pm$

$e = 4pm + 2m$

$f_3 = 4m$

$f_4 = 2m(p - 1)$

When looking at the sphere ($m = 9$, $p = 10$) under a 0.4π-sterad solid angle, thus covering 10% of the sphere surface, we count 22% or 7% of all the vertices, depending on whether the sphere portion's center lies on the pole or on the equator. In addition, a complete surface triangulation is not an intrinsic part of the mesh; after triangulation we count:

$v_{2m} = 2$

$v_5 = 4m$

$v_6 = 2mp - 4m$

So the sphere ($m = 9$, $p = 10$) is meshed with 2 twenty-degree, 40 five-degree and 140 six-degree vertices. Variation of the vertex degree is very important, while in the previous method the number of five-degree vertices remains low and constant.

This icosahedron subdivision sphere generation technique has already been used elsewhere[19] and provides the advantage of a highly uniform vertex distribution on the surface where all faces are of the same degree. This can be helpful for numerous methods based on a surface approach like icosahedral matching,[20] the ellipsoid approximation of protein shape[21] and sphere deflation for solvent accessible surface.[22]

By contrast with Knowlton[23] or Porter,[24] who only memorize the scene portion visible by the viewer, we manipulate the complete three-dimensional object definition. This "brute-force" approach is undoubtedly time and memory consuming, which is why interactive raster graphics require powerful and dedicated hardware.

For a little sphere, namely one filling 1% of the screen area, a first-order icosahedron iteration process approximates the sphere well. For big ones (30% of screen area), a third-order iteration is required to properly fit the surface (Color Plate 3). In molecular drawings one doesn't need to

go very far in the iteration process and depending on whether the picture will be scaled, one can adjust the order to minimize graphic memory space and processing time cost.

Ellipsoid

ORTEP was the first program to allow representation of thermal motion probability ellipsoids on the atomic sites (Figure 2a). Given anisotropic temperature factors, ORTEP computes the principal axes of thermal motion consisting of principal values of RMS displacement and direction cosines for principal vectors relative to the working cartesian system. Two programs developed on a calligraphic display system provide such facility.[7-9] Raster devices allow a more realistic approximation of shaded ellipsoids models to be displayed. We proceed as before but starting from an octahedron. As with ORTEP, octant shading highlights principal axes direction. We achieve this by removing a face and filling the interior with three new faces as shown in Figure 2b.

We first approximate an ellipsoid whose semi-axis lengths are the unit. Then we change orientation and scale according to the given direction cosine and RMS displacement.

ORTEP requires a trial-and-error procedure to find the optimum orientation of the molecule but always tries to orient the ellipsoid octant towards the viewer. Thus, when manipulating the molecules in our program, some octants may not appear when oriented in the same direction as that of the viewer. The solution consists of making two diametrically opposite holes; but this is even less satisfactory when viewing the side of the surface. Therefore the original ORTEP-like representation is kept.

Coordination polyhedron

Rather than a precise determination of the coordination number (CN), we would like to observe the coordination polyhedron (CP) of a given atom. This is a shorthand notation analogous to the organic chemist's use of the hexagon to represent a benzene ring.[25] It is often difficult to compute polyhedron vertices in terms of distances to nearest neighbors. A common example is the body-centered-cubic (bcc) structure in which each sphere is in contact with eight others and has the six next-nearest neighbors at a distance only 15% greater than that to the eight nearest neighbors. Thus, we will not be able to identify a gap in the list of interatomic distances. Frank–Kaspar's proposal[26] is based on the definition of the domain of an atom. It is the innermost polyhedron bounded by planes drawn midway and perpendicular to the lines joining the atom and all other atoms. This procedure defines the Voronoï polyhedron in dual relationship with the coordination polyhedron. However, this definition leads to difficulties in the bcc structure where CN 14 is greater than that of closest packing (12).[27]

In spite of several improvements,[28,29] ambiguities are not removed and automatic generation of any kind of CP seems a tricky procedure to implement. Aslanov and Markov[30] have formally proved that for any interaction potential— provided that the force of repulsion increases when atoms get closer—stable CPs are tetrahedrons, trigonal bipyramids, octahedrons and cubes.
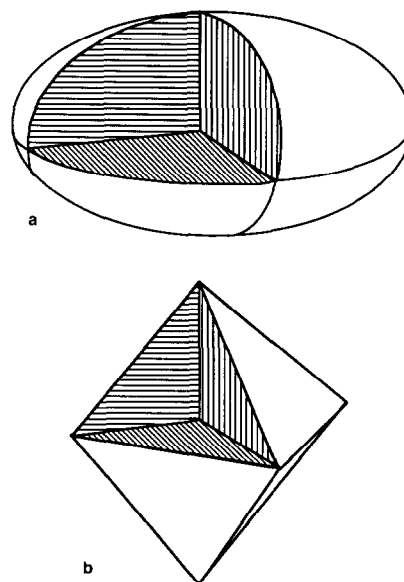

Figure 2. a, ORTEP thermal ellipsoid; b, holed octahedron for approximating the ellipsoid surface

First attempts to represent a polyhedron on a plotter were performed by STRUPLO.[12] This program tries to fit a polyhedron defined by given angle and distance ranges on the central atom; this imposes the knowledge of these values and the trial-and-error procedure is generally required. Second, only tetrahedron and octahedron CP are dealt with because all angles between the central atom and the two incident vertices are in the same angle ranges. Then, trigonal bipyramid is not available. However, this way of doing things allows immediate recognition of the vertex triplet defining a polyhedron face. Whereas with our method, we must organize vertices in such a way that we only extract meaningful triplets.

The importance of the three first CP[25] drives us to generate them automatically. The input data in our procedure are the name of the coordinated atom, a cutoff distance beyond which no neighbor is to be sought and an integer indicating we keep either the 4, 5 or 6 nearest neighbours. Therefore we proceed as follows:

- For the tetrahedron, each vertex triplet defines a face, so there is nothing else to do.
- For the trigonal bipyramid, we look for the two farthest vertices. We suppose that each is the top of one pyramid so it is a three-degree vertex. The three other vertices are the base of each pyramid and are four-degree vertices.
- For the octahedron, the same procedure is applied. We consider the octahedron to be a square bipyramid; but we must yet organize the four base vertices. Here again, the two vertices maximizing the intervertex distance should not be adjacent.

These rules are simple and give good results providing that the square base does not have an edge longer than its diagonal. The coordination number is still an open problem but our program allows one to try several kinds of polyhedral

structures around a given cation until the viewer concludes "this one fits well."

INPUT

X-ray data

In cases where thermal ellipsoids are needed, we retrieve the ORTEP output file that describes them. Because no more graphical orders are needed, very few ORTEP commands are now used. We provide a program to convert a more user-friendly input format to the ORTEP one. This includes Hermann–Mauguin space group symbols and cell parameters, names of the atoms with fractional coordinates and coefficients of the anisotropic temperature factor. The SYMOP program[31] is used to derive symmetry operations from the space group symbol.

For inorganic crystals, we define polyhedrons as described above, giving their color and specifying if they should be affected by a translucency coefficient. The overall connection of new and already existing programs is shown in Figure 3.

Molecules

The SYBYL[6] record format has been chosen as giving all the necessary information for drawing a molecule (atom types and locations, connectivity, bond types, charges and so forth). This format has also been implemented on most available modeling software. The PDB[32] or CCD[33] formats were not retained because no explicit connection between atoms is available.

Dynamics

We use the AMBER[34] format recording the coordinates of atoms in molecular dynamics trajectory. The description of the molecular topology necessary for the definition of bonds comes from a SYBYL input file.

APPLICATION EXAMPLES

Inorganic structures are usually more difficult to visualize than organic ones.[8] All rendering facilities must be enabled to produce accurate and chemically meaningful pictures. The depth-cueing facility is helpful because it smoothly limits the amount of information to analyse. Furthermore, during molecular dynamics animation, it provides information about the z-translation of particles. The clipping facility has been widely used in molecular surface depiction to exhibit cavities, channels and surface contacts between inhibitor and substrate.[35] It is also useful in polyhedral packing: By varying the planes dynamically it highlights edges and shared faces. The shading facility must be applied for surface rendering, but for CP it is often more relevant to disable it; then edges appear clearly. The lighting facility is the last stage of image refinement. Four light source types, controlled by seven coefficients on average, are a very powerful tool but its mastery requires great experience. However, playing with directional light source parameters is a necessary and sufficient condition for inorganic structures.

Inorganic X-ray studies

We are currently studying lithium incorporation in vanadium pentoxide and the first example is taken from this work. In the V_2O_5 structure[36] each vanadium is surrounded with six oxygens. Double chains of edge-sharing octahedra are joined through an octahedra vertex to form layers. The sixth neighbor of vanadium in the adjacent layer is at a distance of 2.8 Å so it is more realistic to describe the coordination as square pyramidal. To achieve this representation we triangulate the square so as to make trigonal bipyramidal and square pyramidal topologically equivalent. While remaining in the application, we can switch between any kind of CP. In Color Plate 1, 90% probability thermal ellipsoids are drawn; oxygen in red and vanadium in grey; the color of each half bond is that of its incident atom, except for the long V–O bond, which is yellow; each vanadium is surrounded with a translucent square-pyramidal. The effect of Color Plate 4 is due to the perspective viewing where the projection reference point is very close to the projection plane. Color Plate 5 exhibits the square-pyramidal sites half filled by lithium in β-$Li_{0.3}V_2O_5$.[37] As in the previous one, β'-$Li_{0.45}V_2O_5$ is a tunnel structure[38] where oxygenated tunnels are parallel to the y-axis, but here all sites are occupied by lithium (Color Plate 6); Li^+ is in a tetrahedral coordination: we used the translucency surface property to exhibit the Li^+ ion enclosed in its CP. Color Plate 7 shows the δ-$Li_{1.0}V_2O_5$ structure.[39]
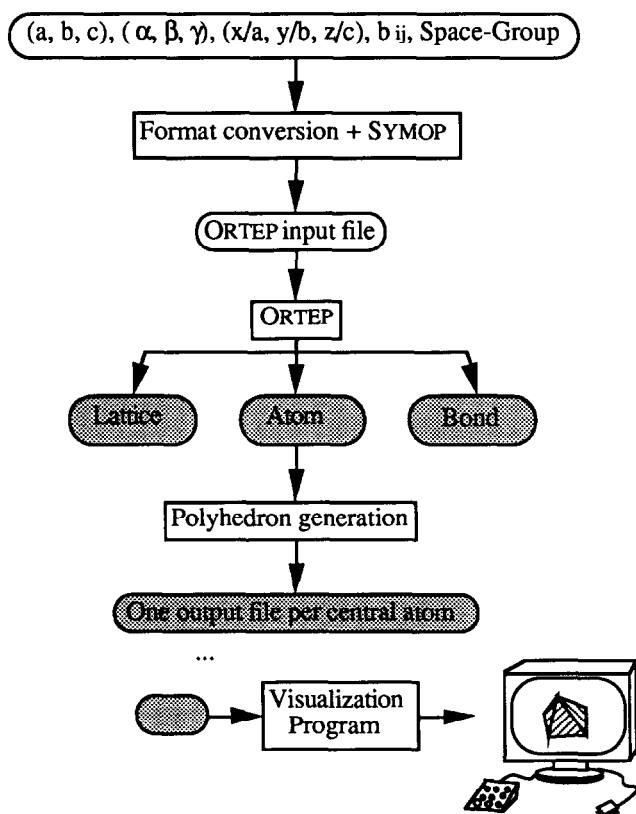

Figure 3. Flow chart for crystal visualization

$(a, b, c), (\alpha, \beta, \gamma), (x/a, y/b, z/c), b_{ij}, Space\text{-}Group$

Format conversion + SYMOP

ORTEP input file

ORTEP

Lattice   Atom   Bond

Polyhedron generation

One output file per central atom

...

Visualization Program

Molecules

Color Plate 8 shows a CPK model representation of the [222, K$^+$] cryptate.

Molecular dynamics

Color Plate 9 is a superposition of 20 conformations of the [222, K$^+$] cryptate[40] obtained from a MD run. Color applied to each vertex of one line corresponds to the bound atom color and a shading method is applied along the line. The potassium ion follows the translucency surface property with bonds appearing behind it.

PERFORMANCES

The first object to be approximated is the sphere. For that purpose, more or less complex original methods have been developed; starting from Porter's scan line depth-buffer[24] through Knowlton's trapezoids decomposition,[23] up to Max's atom cast shading.[41] Most of them are reviewed by Max.[42] Table 1 shows the average speed of recent CPK implementations.

When using a graphic library such as PHIGS, the application is midway between those which are machine dependent [MD], μ-coded or tightly coupled with the hardware, and those which are not [NMD], namely pictures calculated on any mainframe system and output performed on any 8-bit frame buffer with a lookup table.

The execution time of the application includes the execution time of library routines. Both the application code and the PHIGS code should be reviewed for later optimizations. Depending on the complexity of the rendered molecule, we can achieve either real-time manipulation [MD] or static visualization [NMD].

The development and debugging time depends on the user's ability to play with library routines; this is more constraining when one is already mastering another programming language or operating system [NMD]. On the other hand, it's smoother than bending to hermetic formalism of processor μ-codes [MD]. PHIGS provides high-level routines that release the user from large amounts of work (illumination facilities, view transformations, and so forth) allowing him to focus on the development of the application.

The porting time is negligible for NMD applications and there is no reason to run an MD program on a machine for which it has not been designed. Experience shows that porting a library dependant application is only straightforward with the same manufacturer's machine, running the same compiler and the same graphic library version. Porting efforts are proportional to changes level, raising from new library version up to another computer.

CONCLUSION

This paper describes a general visualization and manipulation molecular graphics software. It handles several atomic representations so a wide variety of molecular drawings are performed and applications range from inorganic crystals up to molecular dynamics simulations. We hope that our definition of the general mask is user friendly and efficient for further extensions. A comprehensive vision of polyhe-

Table 1. Speed of CPK drawing

Algorithm used	Spheres/second
Pixel-planes (Special hardware for sphere-rendering)[43]	13000
TAAC-1 (μ-coded on Sun)[44]	1000
DAP (array-processor)[45]	1000
This work	400*
Pique[46]	50
Palmer[47]	50
Max,[41] Cromer[48]	10

*With eight GAP and first-order icosahedron. When about a hundred spheres are depicted, it is more accurate for the viewing to take second-order icosahedron. The interaction times then remain constant

dral packing is also very useful especially for educational purposes, when such arrangements are not readily understandable. This software was used to create a movie representing different aspects of molecular visualization and depicts several LiV$_2$O$_5$ bronze phases. The resultant images are also very beautiful.[49]

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