**CONTRIBUTED PAPERS**

**MOLECULAR MODEL BUILDING AND INSPECTING USING NEWMAN PROJECTIONS AND BIT MAPPED GRAPHICS**

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**Introduction**

Each year more crystal structures are solved, in many cases because chemists or physicists need structural information about compounds and materials they are studying. Then crystal structure determination by X-ray diffraction is the only reliable and relatively fast method, because in a couple of weeks it may produce a three dimensional image of the electron density and thus a unique picture of the molecule.

In the last ten to fifteen years the methods to solve and refine crystal structures from X-ray data have greatly been improved, the computers needed for doing the calculations have gained power, lost weight and increased rapidly in number, and, finally, also the number of sophisticated automatic single crystal diffractometers available around the world is increasing by the year. As a result crystal structures are solved more efficiently, more rapidly, more reliable and more often.

However, the way in which the results of a crystal structure determination are presented is in the same period not very much affected by modern means. Although packages like Mogli and ChemX enable fast molecular graphics, they needs such a sophisticated graphic hardware environment that many laboratories and in particular university institutes cannot afford such a set up. Thus mostly results of crystal structure determinations are presented as atom coordinates, the redundant bond lengths and bond angles, may be some torsion angles and a few figures of the molecule(s), the latter made by means of the famous ORTEP program (Johnson, 1965) or by a more recent plotting program such as PLUTO (Clegg and Motherwell, 1978).

Thus, when for instance an organic chemist likes to study a particular molecule in more detail than is presented in the relevant crystals graphic papers, he needs to learn rather complicated program handling in order to produce plot files himself. For example in our mainframe computing environment one needs to know about the operating system of the Cyber computer, how to handle a graphic terminal such as a H.P., how to input data for ORTEP and PLUTO, and how to send the final results to a plotter. Quite complicated, and not only that, slow as well, because ORTEP and PLUTO can only be carried out in batch mode in view of their core demands. So about 15 to 20 minutes are needed to get a next structural image on the screen and a complete session to get some idea of the structure and a good view direction may take easily as much as a complete afternoon. This in spite of the excellent computing facilities and terminals available in our university. Also the building of a molecular model from atom parameters and cell constants is not a trivial job neither for a chemist, nor for a crystallographer.

In stead, crystallography should provide better tools for chemists to study molecules of their interest in any desired detail. Tools which are easy enough to handle without knowledge of computers or operating systems. Tools, which are also cheap enough to buy them as an add-on, software as well as hardware, without having to worry about budget.

In this paper two tools of this sort are presented. One is realised since a long time in our laboratory and is based on a better way to present torsion angles (Schenk et al., 1985; Brandenburg, 1974). More than bond lengths and angles, it is the dihedral or torsion angles that determine the conformation of a molecule. Consequently Newman projections, which represent graphically all torsion angles around individual bonds, give much more insight in the conformation than tables of bond lengths and angles. By using simple model building kits and a complete set of Newman projections calculated from the atomic coor-dinates any chemist may build in half an hour a
very good resembling model of his molecule of interest.

The second tool makes the use of the first tool userfriendly; it is a menu-driven program for a very cheap home computer, the Commodore 64, by means of which graphical representations can be made at high speed, around one complete drawing per 1-10 seconds. Options of the program are molecular pictures from any view direction in mono and stereo, stick, ball and stick and pseudo-space filling display styles, helping routines for finding a good view, real time rotation of a stereopair, Newman projections, bond lengths and angles, hardcopy facilities. The Commodore 64 including diskdrive, monitor, modem and printer sells for less than $1000; the program is shareware and can be easily handed by chemists, even if they never touched a computer or a computer terminal before.

Throughout this paper all illustrations are just non-retouched hard copies through a cheap graphic printer of the C64 molecular graphics program.

**Newman Projections**

A Newman projection along a bond is a schematic projection of all other bonds which are connected to that bond on a plane perpendicular to it. An example of Newman projection is given in Figure 1, where the staggered conformation of ethane is shown. The midpoint of the circle represents the projection of the particular bond and the projection of all connected bonds are schematically drawn approximately equal in length. Those bonds connected to the first (front) atom are drawn from the midpoint of the circle, and those connected to the second (back) atom from the circle outwards. The Newman projection thus represents graphically all dihedral angles (torsion angles) around a particular bond. Of course, when atom coordinates and cell constants of a structure are known, the Newman projection along all bonds of the molecule can be calculated.

One very important property of Newman projections is their stereospecificity. Whereas bond lengths and angles leave ambiguity regarding the stereochemistry of a molecule, Newman projections are stereochemically specific. They thus can be used to study the stereochemistry of a molecule and moreover, when the absolute configuration of a noncentrosymmetric molecule is determined, the Newman projections also image the correct hand of the molecule.

**Newman Projections in Stereochemistry**

Newman projections are very important to describe the conformation of a molecule. We present three examples here: two from organic and one from coordination chemistry.

**Example 1.**

Whereas the conformation of different steroids might be different because the coupling of successive rings may be either cis or trans, this is not reflected at all in bond lengths and angles. But in case three (but better five) Newman projections are plotted, the differences in configuration between the molecules is quite obvious. In Figure 2 the general numbering of the atoms of the steroid skeleton are given, in Figure 3 the five most important Newman projections of an

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**Fig. 1.** Perspective view of ethane and its Newman projection. Graphics printer plots at 320 x 200 resolution made by MOL64, as other illustrations.

**Fig. 2.** Atom numbering in the steroid skeleton.
Fig. 3. The five most important Newman projections of estrone, showing the prominent features of the geometry of the molecule.

Fig. 4. The same Newman projections as in Fig. 3, now for digitoxine.

Fig. 5. Atom numbering of a four-ring phosphorous compound.

Fig. 6. Stereo pair of the molecule of Fig. 5.
estrone derivative are shown, and in Figure 4 the same ones from digitoxine. By comparing Figures 3 and 4 the big differences in conformation are immediately obvious, whereas the tables of bond lengths and angles (not being reproduced here) are not giving much conformational information at all.

Example 2.

The numbering of the atoms in a compound with four rings coupled to a phosphorous atom are given in Figure 5. Even a stereo pair (Figure 6) does not give exact information about the conformation of the molecule. However, the rings are rigid and just the rotation of the rings around the connecting bond to the central P atom determine the conformation. Thus again, rather than anything else the Newman projections along the four P-C bonds show the geometry of the molecule (see Figure 7). The two-ring system and one of the benzenes are in the planes C2-P2-C21 and C9-P2-C2 respectively, and the two other rings are in planes perpendicular to the planes C15-P2-C21 and C2-P2-C21 respectively.

Example 3.

The last example is a Re-Mn compound from coordination chemistry. The atom numbering is shown in Figure 8, together with the bond lengths and angles regarding the two metal atoms. Again this does not show all details of the complex. However, one Newman projection (see Figure 9) in addition to this and the conformation of the molecule is completely clear. The four perpendicular ligands of the Re atom form a nicely staggered conformation with the four perpendicular ligands of the Mn atom. The four atoms
C6-Re-Mn-C1 deviate appreciably from a straight line with angles at Re and Mn of 171.9° and 162.9° respectively. From the Newman projection it can be seen that these deviations are realised in a plane approximately beseting both N-ligands at Mn, such that C1 is bent away from the N's and C6 in the opposite direction. Again without the Newman projection these details are easily overlooked.

**Newman Projections for Organic Model Building**

Newman projections are much more important to describe shape of organic molecules than all the normally published numbers. This is a result of the fact that changing bond lengths in molecules costs more energy than changing bond angles and in turn changing bond angles costs more energy than changing the conformation (dihedral angles) around a bond.

This implies that the use of standard bond lengths and standard angles and real dihedral angles around the bonds will result in a model resembling well the actual conformation of the molecule. Of course, an improvement is achieved if bond lengths are adjusted to their actual values. This is easily done when straw-like models like Framework Molecular Models (Prentice-Hall, USA) or Orbit molecular building sys-

![Fig. 9. Newman projection along the Re-Mn bond of the complex of Fig. 8.](image)

![Fig. 10. Atom numbering in a two-ring compound.](image)

**Table 1. Bond lengths and angles for all atoms of the molecule displayed in Figs. 10 and 11. In model building this is used to cut bond lengths and select the most resembling standard bond angles.**
tem (Cochranes of Oxford, UK) are used. In these kits there are a number of different standard angles available and for each atom the most alike has to be chosen.

An example of a not to complicated molecule is presented in Figures 10 and 11 and Table 1 although it may be noted that more complicated molecules are not more difficult to handle; it is just more time consuming. Atom numbering is given in Figure 10, bond lengths and angles for each atom in Table 1, and all relevant Newman projections in Figure 11. As can be seen easily from Figure 10, the conformation of this molecule is not very easy to follow because of the seven membered ring and its side chains, two of which are rather free to settle their conformation.

To build the model now first for each of the atoms an appropriate angle-connection is selected from the kit using Table 1. So for Cl a 3-way with angles of 120°, for C2 a tetraeder, for C3 a 3-way with 120° angles, etc. Then for each of the bonds straws are cut at the desired lengths. After a scale for the model has to be decided on, e.g. 1 Å = 2.5 cm, because this approximates 1 Å to 1 inch and consequently all over the world this scale is a convenient one. Now the actual model is assembled using the Newman projections to settle the dihedral angles roughly. When this is finished once more all Newman projections are inspected and where necessary fine tuning of the dihedral angles has been carried out. This is easiest done by taking the model in the same orientation as the Newman projections and adjust the angles of the model visually to those of the Newman projection. After this second cycle of Newman projection use the model is ready and well resembling

Fig. 11. All Newman projections of the compound of Fig. 10, with exception of those regarding the benzene ring (C14-C19) which just show torsion angles of 0 and are not necessary to build the model of the molecule.
the true molecular structure as found from the crystal structure determination.

Future Changes in Crystallographic Computing

To introduce the second tool for molecular inspection and molecular graphics, first a trend in computing will be signalized.

As already mentioned crystallographic computing has contributed a lot in the improvements of crystal structure determination and will do in the next future. However, it will also change its character as a result of distributed computing and local area networks, and as a result it will be easier to access for developing countries as well.

Traditionally crystallographic methods are implemented either on mainframes or on mini's, the latter generally controlling at the same time an automatic diffractometer. Mostly multi-user systems make it possible that many users run their jobs through video terminals in competition with each other. When the computer is too busy, this implies that every user is equally discontented. Modern computer hardware technology, however, will make it possible soon that for the price of a video terminal one gets a remarkably powerful computer on the desk. When these com-puters are connected in a network than many of the jobs now carried out on mainframes rather will be done by the local desk-top computers and the main-frames will be used for special purposes only. Of course, also stand-alone the desk top will be a useful tool in particular in those countries where mainframes are scarce.

Part of this future development could be realised already now, because the IBM AT's, Commodore Amiga's, Atari 1040's, Apple MacIntosh's and others comprise already impressing computing power. A few years ago it was already shown that even on an 8-bit microcomputer (TRS80) structure factor least squares refinements could run efficiently (Loopstra et al., 1982). Typically by the TRS80 a 25 atom structure is being refined from $R = 35\%$ to $15\%$ in around 1 1/2 hours.

Certainly within a few years many of the calculations involved in crystal structure determination will be possible on desk top machines because appropriate software will be developed.

If one looks for graphic power alone, than it is very impressing to see what cheap machines like the Commodore 64 and the Sinclair Spectrum achieve in the field of animated computer games for children and for those who call themselves adults. Therefore when we were looking into the possibility to improve our molecular graphics situation from the one as described in the introduction to a more modern one, it was natural to look into the possibilities of Commodore 64 with its monochrome 320 by 200 bit mapped graphics, for which not only Basic interpreters are available, but also Basic compilers. It appeared to us lately that even molecules with as many as 200 atoms will give a stereo pair of good resolution. In our laboratory also a MS-DOS version has been written, for which the 640 x 200 resolution gives the same image quality as the C64 because the pixel-size is rectangular, and thus also in this case rather 320 x 200 with its square pixel size determines the resolution of the pictures.

Raster Graphics on Cheap Microcomputers

Of course all plotting programs such as ORTEP are line or vector oriented. When a line is plotted on a piece of paper it is definite and cannot be removed, so line pieces which should be hidden by bonds or atoms more in the foreground of the picture have to be calculated first and are successively not being drawn.

In bit mapped or raster graphics pixels are either on or off, so when one starts drawing a picture from farthest away to nearest no hidden lines have to be calculated because pixels may be set and reset as many times as necessary to give the final picture. With raster graphics also easily solid atoms can be imaged. However, to get good resolved 3-D space-filling models one needs at least 32 different tones of grey or of another color in order to shade in a realistic way. With our cheap monochrome possibilities this of course cannot be achieved.

The speed of the program depends in general on the speed by means of which bits in the graphics memory are set to 1 and reset to 0. We started using the rather slow Simon's Basic routines (Basic extension of CBM), however, since we just draw lines and circles later some small resident machine language plotting routines have been written, which speed up the program in particular when large solid atoms are drawn.

The Graphic System

The system has been developed in the Basic 2.0 interpreter, but is used in the compiled version (Data Becker Basic 64) for a speed increase of roughly seven. It is run by simply typing two commands (LOAD, " * ", 8 and RUN) and from then on it is completely menu-driven for user-friendliness. (The MS-DOS version has an autoloader). The main menu
contains seven options: 1. manual; 2. input editor; 3. a terminal-based input editor; 4. molecular graphics program MOL64; 5. real-time molecular rotation ROTMOL64; 6. directory display of PLOT; 7. copyright information.

The manual can be displayed or printed, the copyright information gives all details about the shareware character of the program.

The input editor is a line oriented dialog type editor which makes it easy to produce a complete plot-file from the data of a crystal structure which can be used successively in both the molecular graphics routines ROTMOL64 and MOL64. This option is used to input structures from literature to modify existing parameter files or when no main frame is available.

Another editor is present, the terminal editor. By means of this one, the C64 is logged in on the host, the cell constants and atom labels and coordinates are prepared in the host editor, and then downloaded to the C64, after which the rest of the plot-file is again being prepared in dialog with the C64.

The directory option just displays or prints a subdirectory of all labels of the different plot-files available on the diskette.

MOL64

The molecular graphics program has been designed to enable as much as possible the simultaneous use of any graphical and numerical information; in particular the display of Newman projections and bond lengths and angles are included on top of the following options:

To display the molecule as stick model, as ball and stick model or as ball (or rather disk) model, in mono-, or stereo-view, with or without labels. The model can be rotated in three dimensions. To help to find a good view a least squares plane can be calculated through any numbers of specified atoms and also a "minimum" overlap view. The view matrix is identical to that of PLUTO and can be displayed at any moment. Also the relevant input data for ORTEP can be displayed. Hard copy images of molecules and of Newman projections can be made by the normal cheap printers in graphic mode (e.g. the MPS 803) and on the output the relevant data regarding the view direction are also printed.

All standard default-settings can be changed. So e.g. the bonds in the molecule are found by the program through search radii; de default-values of these radii are those as available on the parameter file,

![Fig. 12. Mono printer plot of the Re-Mn compound of Fig. 8. Standard the three rotational angles are printed in all molecular hard copies, to serve as a reference for PLUTO plots.](image1)

![Fig. 13. Pseuo-spacefilling model of the Re-Mn compound.](image2)

![Fig. 14. Stereo pair of a pseudo-spacefilling model of a more-ring compound, with and without hydrogen atoms.](image3)
but in the edit menu they can be changed as to include more or fewr bonds in the drawings. This applies also to plot radii, the settings of screen and drawing and to the focus and eye distance for stereo pairs. For example by changing the eye distance to a negative value the left and right images are interchanged, so that for people who can see stereo without any means (viewer) right from the screen (50% of all people), not only those who look parallel are served, but also who look crosswise.

Most functions can be reached by hitting one key; now and then the program asks then for additional information, such as the angle to rotate. Then a number is typed on the keyboard followed by return upon which the computer does the calculation. Any key without a meaning which is touched displays the menu.

The output of many of the options are already familiar to the reader through the hard copies used in the preceding paragraphs. A few additional ones may, be presented here. In Figure 12 a ball and stick mono view of the Re-Mn compound together with the view direction information and in Figure 13 a pseudo-spacefilling picture of the same compound. Figure 14 shows pseudo-spacefilling stereo pairs of a complicated many ring system with and without hydrogen atoms. Figure 15 shows two stereo views of the stick model of the phosphorous four-ring system of Figure 5 and finally in Figure 16 a 130-atom asymmetric unit is shown in several display styles, which is the largest structure we tried up till now.

**Working with MOL64**

The performance of MOL64 is good; where in our university a coworker spends an afternoon at a
graphics terminal of the mainframe to get a good view of his molecule of say 30 to 40 atoms, at the CBM64 graphics subsystem this is reduced to about a quarter of an hour. The most time consuming operation is the calculation of the minimum overlap view which takes about half a minute for a molecule of that size. Rotation and display of a stick model is a matter of seconds. Ball models are also more time consuming, but seldomly the drawing of a picture will take longer than 10 seconds.

**ROTMOL64**

The real time rotation program ROTMOL64 rotates and displays permanently a stereo pair of the molecule: figure 15 can be considered as two snapshots of the screen of the monitor. The functions of ROTMOL are also activated by hitting a single key. The molecule can be zoomed in and out; rotate faster or slower; the two pictures display normally for parallel stereo, however for "cross-lookers" they can be interchanged; the distance between the pictures can be changed such as to fit for a local stereoviewer; rotations may be around \( x \) (horizontal screen axis), \( y \) (vertical screen axis) and \( z \) (perpendicular to the screen).

The performance is such that for a 30 atom structure approximately one picture per second is generated. Two bit planes are used, one for drawing and one for displaying, and they are interchanged when the drawing is ready.

**Model Building with MOL64**

The model building by means of Newman projections is very easily done with the assistance of MOL64. After inputting the cell constants and atom parameters via the editor or via a mainframe link, first a printer plot with labels is made and all distances and angles are inspected one by one to find out the bondlengths to be used and the most resembling standard bond angles. Now a rough model can be assembled from straws/standard angle connections. Fine tuning follows by rotating all conformations around individual bonds such that the dihedral angles reflect the respective Newman projections calculated with the program. The result is a well resembling model. In the University of Amsterdam (Driessen et al., 1986) first year chemistry students learn in this way successfully to build a model from the data of a randomly chosen Acta Cryst. paper. They quickly explore all possibilities of the program and moreover they get better models to study. In the course Chemistry I of the Dutch Open University this model-building procedure is taken up as one of the Computer Assisted modules (Schenk, 1985) in a specially written MS-DOS form.

**References**


