Simple and efficient approach to preparation of molecular drawings

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A convenient approach to the preparation of good quality molecular drawings is described. The method is based on transforming the atomic coordinates provided by a conventional crystallographic structure analysis or deduced from a model of a particular molecule, to a suitably weighted molecular inertia system and forming a projection of the molecule down the axis that corresponds to its highest moment of inertia. When implemented in a routine which prepares the input to the program ORTEP, the new method very nearly eliminates trial-and-error procedures from the preparation of a molecular diagram with suitable orientation of the molecule.

Keywords: molecular graphics, weighted molecular reorientation, ORTEP, PREORT

received 20 April 1984, revised 14 June 1984

The automatic preparation of molecular drawings of presentable quality requires that: (i) a flexible and general plotting routine is available, (ii) the requirements posed by the preparation of the input data should be modest, so that users from various disciplines can cope with them and (iii) that the desired orientation of the molecule should be achieved with as small a number of trials as possible.

The first of these demands is met by a variety of computer programs. Of these the well-known crystallographic program ORTEP[1] is the most widely used, and it is frequently quoted in the literature. However, the input to this flexible routine is, or appears to be, rather complicated for users who are not accustomed to crystallographic terminology. Moreover, the selection of the line of view, for which most parts of a molecule will appear unobscured by overlap, usually requires several trials and may become time consuming unless expensive graphics equipment with on-line orientation control is available.

Since these practical disadvantages appear to the author to be outweighed by ORTEP's performance with a conventional off-line plotter, it was decided some years ago to resolve these problems by (i) constructing a routine with input requirements more suited to the general user, and which preprograms the input to ORTEP and (ii) taking care of the orientation–overlap problem by making use of the properties of the tensor of inertia[2] and the effect of the choice of atomic 'weights' on the orientation of its eigenvectors. The minimum hardware requirements are a computer on which ORTEP can be run, and a conventional plotter.

The minimum-overlap projection of a molecule is its best plane and the corresponding plane normal is usually close to an eigenvector of the molecule's tensor of inertia and is exactly so if all the atoms are assigned equal weights[3]. To produce this projection, the atomic coordinates are transformed to an arbitrary Cartesian system and the molecular tensor of inertia is constructed and diagonalized. An appropriate transformation is then applied to the atomic coordinates (and to the vibration tensors[4] if the display of thermal ellipsoids is also desired). The key feature of the approach here is the choice of atomic 'weights' in the construction of the tensor of inertia: the weighting of atoms in an illustration seems to be a powerful substitute for orientation changes by successive rotations, as shown by the example below.

The method outlined above is illustrated by the preparation of an ORTEP drawing of Siphonochalin acetate[5]. This is a derivative of a natural (marine) triterpene and its complicated conformational detail would require a number of trials for a graphical illustration to be formed in the conventional manner. Instead, a best-plane projection of the molecule is first constructed with all the atoms being given unit weights. The result, shown in Figure 1, shows most of the molecular structure but it is still unsatisfactory since part of the molecule is hidden by overlap. This initial projection

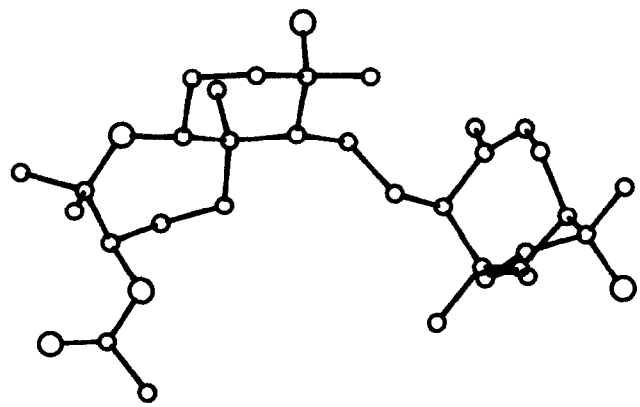

Figure 1. Equal-weight projection of Siphonochalin acetate[5]. The small circles denote carbon atoms, and the larger ones oxygen atoms

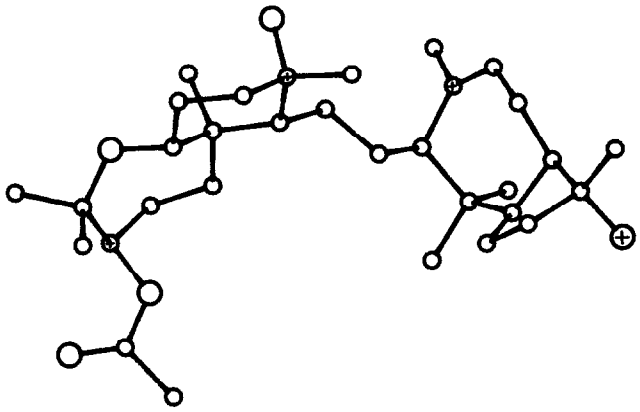

Figure 2. Weight-controlled reorientation of Siphonochalin acetate[5]*. The input for the preparation of Figure 2 is the same as that used for Figure 1, except that the atoms denoted by crosses are given high weights (1000 units) (see text)*

can be improved by rotations about the horizontal and vertical axes of the plot, but a single weight-controlled reorientation gives the unobscured view of the molecule shown in Figure 2. Figure 2 was constructed by assigning to the atoms marked by crosses, weights of 1000 units, while leaving unit weights on the remaining atoms.

The input routine described above, called PREORT, has been operating in conjunction with ORTEP on a CDC mainframe at the Tel Aviv University for a few years, and has been of use to crystallographers and non-crystallographers alike. There seems to be no restrictions that might prevent adapting it to a mini- or microcomputer for which a version of ORTEP is available.

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