

## TEACHING STEREOCHEMISTRY WITH COMPUTER GRAPHICS

by Richard E. Partch\*

Teaching molecular stereochemistry at Clarkson has taken a quantum leap forward as a result of the University's commitment to computer-based education. Commencing in the Fall of 1983, all entering freshmen received a Zenith computer. Thus, each student now has in his/her room the necessary hardware for using or creating software.

Prior to the release of the model 200 computer in mid-1986, very little educational software was commercially available for use on the Zenith. As a result, it was necessary for Clarkson faculty and students to write programs for use in study and research. One example, titled "Molecular Stereographics", was developed by three undergraduate computer science majors and myself. This software provides the user much more structural information about molecules than most other commercial programs written for use with the Apple and IBM PC's. Data has now been accumulated on the successful use of such software to enhance student understanding of molecular stereochemistry. In order to make this software more universally attractive, an IBM-PC compatible version was developed. (Professor O. B. Ramsay, Head, Department of Chemistry, Eastern Michigan University used the software to teach stereochemistry in China the Fall of 1986.) Brief descriptions of the stereochemical operations which can be performed and the type of study questions that have been assigned for students to solve are described below.

Table 1 lists the commands a user has at his/her disposal. Several commands are the same as those in software previously written by others, but, this stereographics program also allows one to

- 1) obtain interatomic distances (ethanol, Fig. 1)
- 2) view single, double and triple bonds as one, two and three lines, respectively (3,5-dimethylbenzotrile, Fig. 2)
- 3) view in Newman or sawhorse projection conformational rotation about any bond ( $C_2-C_3$  of propene, Fig. 3-4)
- 4) observe dihedral angle values for any pair of atoms while bond rotation is taking place
- 5) view a molecule and its mirror image at the same time and carry out any of the commands on either (trans-3-chloro-methylcyclopentane, see cover)
- 6) observe and carry out commands on two different molecules at the same time (butane, chloroethene, Fig. 5), and
- 7) delete one peripheral atom from each of two molecules in view and combine the remaining fragments to create a new, single molecule (1-hydroxyethyl + cyanomethyl — 2-hydroxypropionitrile, Fig. 6).

A series of instructional pages are included in the software which describe, among other things, the 25 different elements that may be used to construct molecules (e.g., C, Li, B, Mg, Si, Fe, Pt, Eu), the 18 molecules already entered into the directory (Table 2), and the method of entering new molecules for stereographic study.

The software has been used over a two year period by 230 students in four different classes studying first semester organic chemistry. In every class, the average on quiz and exam questions dealing with stereochemical concepts, (e.g. chirality, conformation, unimolecular and biomolecular reaction mechanisms) was at least 12 points higher than the average on similar questions obtained in 12 years of teaching without graphics software. At the beginning level, the computer graphics program is apparently far better to learn from than student molecular models, possibly because molecules viewed and manipulated on video are more closely related to the format on written exams.

All students are asked to view aspects of the stereochemistry of several molecules already in the directory. Homework may include assignments like: 1) What is the dihedral angle relationship between the chlorine and nitrogen atoms in 2-chloroacetaldehyde imine? 2) Print out the highest and lowest energy Newman projections of ethyl-hydrogenperoxide about the C-O bond. 3) What is the interatomic distance between the  $C_4$  ring carbon and a hydrogen on the methyl group attached to boat cyclohexane? 4) Construct a chiral molecule from any pair of non-chiral molecules and then print out the side-by-side view of the enantiomers of the molecules before and after they are overlapped to show non-superimposability.

After the student becomes familiar with the software by using the seven stereographic manipulations listed in the instructions and doing the homework described above, each student is assigned three unique molecules to enter into the directory of his/her disk. Examples of these assignments are: 2-chloropropane (least stable eclipsed) trans-2-bromo-methylcyclopentane, p-toluic acid; cyanogen, 1,3-dimethylcyclohexane (most stable), triphenylphosphine; diethylpropylboron, cis-ethylenediaminedichloroplatinum, europium acetylacetonate. Successful completion of this part of the homework requires each student to understand the relationship

TABLE 1

Press any key to view molecule again.

<b>Movement Commands</b>	<b>Transpose Commands</b>
(X) X Axis Rotation	(T) Transpose
(Y) Y Axis Rotation	(M) Mirror Image
(Z) Z Axis Rotation	(Q) Quit Transposing or Mirror Image
(-X) -X Axis Rotation	
(-Y) -Y Axis Rotation	<b>Miscellaneous Commands</b>
(-Z) -Z Axis Rotation	(D) Interatomic distance
(R) Bond Rotation	(A) Dihedral Angle
Up (U) Down (D)	(C) Atom Deletion
Left (L) Right (R)	(K) Molecular Bonding
	(E) Exit
<b>Display Commands</b>	(H) Halt
(I) In	(HELP) Help
(O) Out	(S) Speed
(S) Stick	
(G) Globes	
(F) Full	

Use capital commands for large movements, lower case for short movements.

FIGURE 1

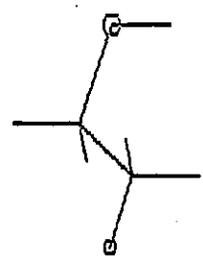
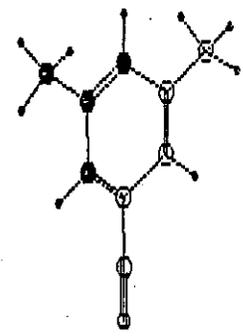


FIGURE 2



Distance equals 3.36

TABLE 2

3. THE DIRECTORY. The directory lists the file names for eighteen varied molecules already entered onto the disk. They are:

ETHANECL.REP	ethane (eclipsed)
ETOH.REP	ethanol
ETHPEROX.REP	ethylhydrogen peroxide
CLETHENE.REP	chloroethylene
CLACETIM.REP	2-chloroacetaldehyde imine
ACETCN.REP	acetonitrile
BRACET.REP	bromoacetone
PROPEN.REP	propene (eclipsed)
CLPROCN.REP	2-chloropropionitrile (most stable eclipsed)
BUTANE.REP	butane (staggered)
CLNECYP.REP	trans-3-chloro-methylcyclopentane
BRCYHEN.REP	cis-1,2-dibromocyclohexane (most stable chair)
CYHXB.REP	methylcyclohexane (boat)
BICYCLO.REP	bicyclo(2.2.1)heptane
CLMEBEN.REP	1-chloro-3-methylbenzene (m-chlorotoluene)
HOSY.REP	o-hydroxystyrene
DIMEBEN.REP	3,5-dimethylbenzonitrile
TYLENOL.REP	tylenol

FIGURES 3-4

Dihedral angle =

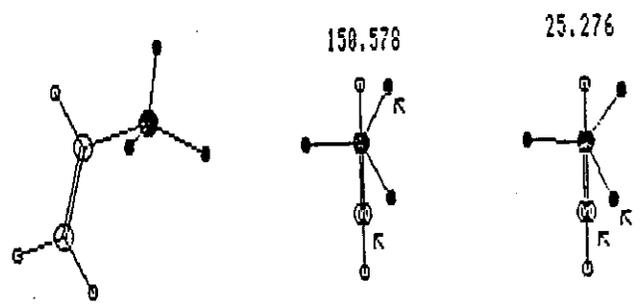


FIGURE 5 (ALSO SEE COVER)

FIGURE 7

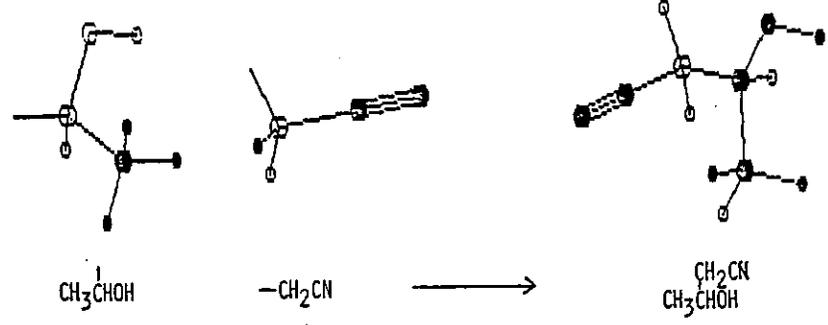
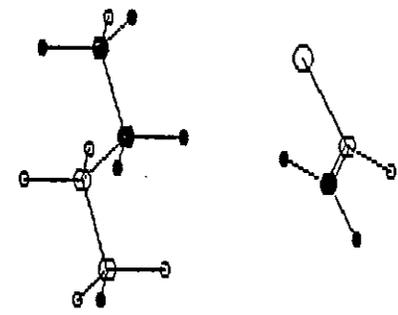


FIGURE 6



between bond lengths, bond angles and dihedral angles when representing a molecule in three dimensions. Disks are collected and evaluated to determine if the student has entered the molecules correctly.

In summary, there is strong evidence that students of organic chemistry substantially enhance their understanding of molecular structure when they are assigned computer graphics homework. Therefore, whenever possible, instructors should incorporate such software in their courses. In fact, the stereographics program we have developed has application even in freshman college and high school advanced placement courses.

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