GRIMM — an interactive personal-computer graphics interface to molecular mechanics

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GRIMM, an interactive personal-computer graphics program designed to be used as an interface to the molecular mechanics program MM2, is described. It facilitates the interactive preparation of input data for MM2 and the visualization of the resultant structure. GRIMM can also be used to construct, modify and manipulate molecular structures shown on a screen.

Keywords: personal computer, computer graphics, molecular mechanics, molecular modelling

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Molecular mechanics calculations have recently found wide use, particularly in the field of organic chemistry and drug design[1–6]. At present, they have limited applications but in spite of this, they are the most practically convenient methods for predicting stable conformations and their energies of organic molecules some with as many as several hundred atoms. Molecular mechanics calculations require first a manual input of coordinate data and atom connection lists for a trial structure of the molecule, usually ascertained from a molecular model, but this is often tedious and time-consuming work. In addition, it is not easy to know whether the input data actually represent the trial structure, and to know what structure the output data represent, unless an appropriate molecular graphics system is available.

To eliminate these problems, we have created an interactive molecular graphics program, GRIMM, for a personal computer. GRIMM is designed to be used as an interface to Allinger's molecular mechanics program MM2[7], since MM2 is the most general, the best tested, and the most widely used of various molecular mechanics programs. GRIMM can also be used as a standalone molecular modelling program.

A number of molecular graphics programs for personal computers have been reported[8–19] and we have utilized some of them[14,18] in GRIMM. Powerful molecular modelling programs, for example, MMMS[20] and NAMES[21], have already been developed for largescale computers. Recently, Liljefors reported the program MOLBUILD[22] for a minicomputer. The purpose and functions of this program are similar to those of GRIMM. One of the main differences between MOLBUILD and GRIMM is that GRIMM runs on a low-cost personal computer. Other features of GRIMM will be demonstrated below.

IMPLEMENTATION

We used a 16-bit personal computer, the NEC PC-9801 (RAM 128 kbyte), equipped with a colour character display, the NEC PC-8853n, with an 8 in floppy disc drive unit, the NEC PC-9881, and a printer, the NEC PC-PR201. The PC-9801 was connected to a HITAC M-280H computer of the Computer Centre, University of Tokyo, through an RS-232C interface. The molecular mechanics program MM2 is stored on the HITAC machine as a library program of the Computer Centre.

OVERVIEW OF GRIMM

Program organization

GRIMM is composed of two program modules: the main program GRIMM.MAIN and the molecular-model-building program MOLDA4. They are written in N_{88}-Basic(86), and are totally interactive. When GRIMM.MAIN is loaded and run, the following five options are shown on the main menu: (1) read molecular structure data from a floppy disc; (2) call MOLDA4; (3) display a molecular structure model; (4) convert data between MOLDA4 and MM2; (5) end. The desired option is selected by entering the option number. Those options except (2) can immediately be put in operation. When option (2) is selected, MOLDA4 is called and the following three options are shown on the main menu of MOLDA4: (1) read molecular structure data from a floppy disc; (2) make molecular structure data; (3) end. When the session of MOLDA4 ends, GRIMM.MAIN is called and its main menu appears. Although MOLDA4 is usually called from GRIMM.MAIN, MOLDA4 can also be used as a standalone molecular-model-building program. The present version of GRIMM can deal with up to 300 atoms and 300 bonds.

Session with MOLDA4

When option (2) of the main menu of MOLDA4 is selected, all of the commands of MOLDA4 (Table 1) are allocated to function keys and these allocations are

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Table 1. Commands and subcommands in MOLDA4

Command	Subcommand	Description
input	atom	Input the number of atoms, the atomic coordinates, and the atomic numbers
	bond	Input the atomic connection list
	alkane	Make the all-*trans* conformation of an *n*-alkane by input of the number of carbon atoms
	hydro	Add hydrogen atoms to the carbon atoms
	a-No	Replace a specified atom by another atom
cancel	atom	Delete a specified atom
	bond	Delete a specified bond
	compo	Delete a specified group of atoms
merge	point	Place a molecule read from a floppy disc with a specified atom at a specified position
	atom	Replace an atom or group of atoms of the molecule by a single atom or group of atoms obtained by abstracting a specified atom from molecular data read from a floppy disc
	bond	Connect two molecules in such a way that their specified bonds overlap
	subst	Substitute an atom or group of atoms with a common substituent
group	C*n*	Do operation C_n
	M	Do operation σ
	I	Do operation i
	S*n*	Do operation S_n
move	atom	Move the origin to a specified atom
	middle	Move the origin to the midpoint of two specified atoms
rotate		Do a whole rotation about a specified coordinate axis or an internal rotation around a specified bond
window	right	Move the viewpoint to the right
	left	Move the viewpoint to the left
	up	Move the viewpoint up
	down	Move the viewpoint down
	zin	Zoom in
	zout	Zoom out
print	print	Output the molecular structure data to the printer
	copy	Output the hard copy of the graphics display on the screen to the printer
save		Save the data on a floppy disc

indicated on the screen for each function key. Selection of a command activates the corresponding subcommands.

The input of molecular structure data is commenced with the 'input' command. Input data are Cartesian coordinates of atoms, atomic numbers and atom connection lists. The all-*trans* conformation of an *n*-alkane can be generated in a one-step operation using the 'alkane' subcommand. The input structure need only be a carbon skeleton as hydrogen atoms can be added to the skeleton using 'hydro'. A specified atom may be replaced by another atom using the 'a-No' subcommand.

The resultant molecule is displayed as a wire model on the graphics screen. The molecule may be rotated (whole rotation or internal rotation) using the 'rotate' command and moved by 'move'. The molecule may be viewed along any of the coordinate axes by using the 'window' command. Specified atoms, bonds and groups of atoms may be deleted using the corresponding subcommand of 'cancel'.

Any molecules made by MOLDA4 can be connected with each other using the 'merge' command. This is an interesting feature of MOLDA4. There are four modes of merging. Using the 'point' subcommand, for example, a supposed structure such as a catenane or a transition state may readily be made (Example 1 in Figure 1). Two molecules can be connected by the use of 'atom' (Example 2 in Figure 1). Two ring systems can be fused using 'bond' (Example 3 in Figure 1). Substitution with a common substituent may also be implemented with 'subst' (Example 4 in Figure 1).

A second interesting feature of MOLDA4 is the 'group' command. By using its subcommands, the corresponding 'symmetry operation' can be performed. The symmetry operations are defined as follows: operation 'C*n*', for example, is defined as to cause the molecule to have a C_n symmetry axis (Example 5 in Figure 1). Thus, the amount of input data may be reduced. It is worth mentioning that the construction of a complicated molecule such as coronene is greatly simplified using this operation.

The molecular structure data may be printed out on a printer using the 'print' subcommand of the 'print' command. The data may be transferred to a floppy disc using the 'save' command. The data on a floppy disc may be read from MOLDA4 or GRIMM.MAIN. A hard copy of the image on the graphics screen may be produced on a printer using the 'copy' subcommand of 'print'.

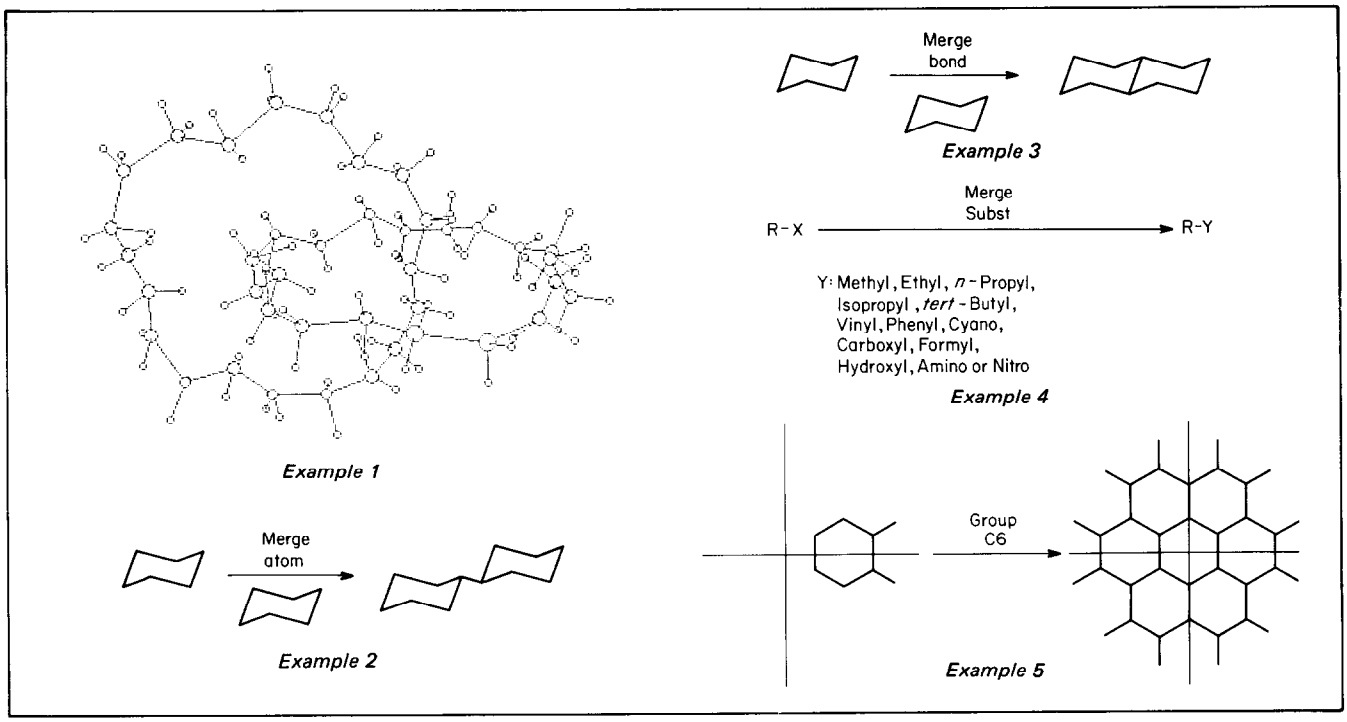

Figure 1. Molecular modelling with MOLDA4. (Example 1) Catenane of two cycloicosane molecules. (Example 2) Construction of bi(cyclohexane) from two cyclohexanes. Any conformation may be made by specifying which bond is involved in the substitution and by specifying its dihedral angle. (Example 3) Construction of decalin from two cyclohexanes. The cis*-isomer, as well as the* trans*-isomer, may be made by specifying which bonds are involved in the ring fusion. (Example 4) Substitution with a common substituent. (Example 5) Construction of coronene from benzene*

Session with GRIMM.MAIN

When option (3) of the main menu of GRIMM.MAIN is selected, the molecular structure constructed by MOLDA4 may be displayed as a wire or a ball-and-stick model. A stereoview of the ball-and-stick model may also be obtained. Interconversion between two structures such as in the nitrogen inversion in piperidine may be visualized in a two-frame animation using the 'anima' command. Using 'analy', the coordinate data of atoms, the distance between any two atoms, bond angles and dihedral angles can be calculated.

When option (4) of the main menu is chosen for input of data to MM2, the following four options are shown as a submenu: (1) make data for molecular mechanics; (2) transfer data between host and terminal; (3) read molecular mechanics data; (4) end. By selecting option (1) of the submenu, the molecular structure data made by MOLDA4 are converted into MM2 input data. In MM2 an atom is specified with an 'atom type' instead of an atomic number. An atom specified with an atomic number is usually classified into several atom types depending mainly on its orbital hybridization. In the data conversion from that for MOLDA4 into that for MM2, each atomic number is transformed into the default atom type shown in Table 2. Other atom types are specified by the use of the 'TGO' command. The MM2 input data saved on a floppy disc may be transmitted to the computer on which the MM2 program is stored by invoking option (2) of the submenu. When the MM2 calculation is completed, the MM2 program produces, in addition to its standard output, a small file with refined Cartesian coordinates and a bond table. This file is transferred to the personal computer and is saved on a floppy disc. The data in this file are converted into the data for GRIMM by using option (3) of the submenu. As a result, the molecular structure data refined with the MM2 calculations may be visualized and they may also be used as good starting data for the next molecular-model-building session.

Table 2. Default atom types in the conversion of data for MOLDA4 into that for MM2

Atomic number	Atomic symbol	Atom type in MM2
1	H	5 Hydrogen atom of C–H bond
5	B	26 Trigonal boron atom
6	C	1 Tetrahedral carbon atom
7	N	8 Pyramidal nitrogen atom
8	O	6 Oxygen atom of C–O–H or C–O–C bonds
9	F	11 Fluorine atom of C–F bond
14	Si	19 Silicon atom of silanes
15	P	25 Phosphorus atom of phosphines
16	S	15 Sulphur atom of sulphides
17	Cl	12 Chlorine atom of C–Cl bond
35	Br	13 Bromine atom of C–Br bond
0[a]	LP	20 Lone pair

[a] A lone pair is treated as an 'atom' of atomic number 0 with atomic symbol LP in GRIMM.

CONCLUSION

Using this system: (1) the labour involved in preparing molecular structure data and the MM2 input data is substantially reduced and (2) the perspective of a molecular model is readily obtained. With the addition

of small program modules, this system may be connected with a variety of programs other than MM2, such as molecular orbital calculation programs, and hence it may be utilized as a versatile tool in various fields of chemistry.

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