MOLDA for Windows – A Molecular Modeling and Molecular Graphics Program Using a VRML Viewer on Personal Computers

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MOLDA for Windows, an interactive personal-computer molecular modeling and molecular graphics program, which can be used as an interface to the ab initio molecular orbital program GAUSSIAN 94, the molecular dynamics simulation program AMBER 4.0 and the molecular mechanics program MM2, is described. The molecular model constructed by using MOLDA can be transferred to the Virtual Reality Modeling Language (VRML) format file and viewed by using a VRML viewer on the World Wide Web (WWW).

Keywords: Molecular modeling, Molecular graphics, World Wide Web, Virtual Reality Modeling Language

1. INTRODUCTION

Molecular modeling and molecular graphics using personal computers have been developed dramatically during the 1980–1990’s. In the 1970’s, powerful molecular modeling programs were developed only for large-scale computers [1,2]. In 1984, interactive molecular modeling programs, MOLDA and GRIMM, on personal computers for interface to molecular science were developed [3]. These programs were designed to be used as an interface to Allinger’s molecular mechanics program MM2 [4], since in those days, MM2 was the most general and widely used program in chemistry. In recent years, however, ab initio molecular orbital (MO) calculations and molecular dynamics (MD) simulations have been widely used, not only in theoretical chemistry but also in organic chemistry and drug design.

The recent development of the Internet, especially World Wide Web (WWW), has changed the computer network and computer graphics dramatically. For three-dimensional (3D) graphics on the computer, the Virtual Reality Modeling Language
(VRML) is used on the WWW. Molecular graphics using VRML has also been developed recently [5,6]. This new technique enables us not only to display molecules on the screen but also to change the point of view with respect to the object shown.

Under such circumstances, we have developed an interactive molecular modeling and molecular graphics program MOLDA for Windows, which is designed to be used as an interface to the ab initio MO program GAUSSIAN 94 [7] and the MD simulation program AMBER 4.0 [8] as well as the molecular mechanics program MM2 [4]. The 3D molecular structures in VRML format can be generated by using this program and the molecular models are exported over the Internet by using VRML.

2. IMPLEMENTATION

We used an IBM/AT compatible (DOS/V) machine, in which the Microsoft Windows95/NT3.51 operating system was installed. The MOLDA for Windows was written in Microsoft Visual Basic 4.0. A Netscape Navigator which plugged-in a Live3D was used as a VRML viewer. The DOS/V machine was connected to UNIX workstations through TCP/IP protocol. The ab initio MO program GAUSSIAN 94 and the MD simulation program AMBER 4.0 were used on these workstations.

3. OVERVIEW OF MOLDA FOR WINDOWS AND DISCUSSION

3.1. The Feature of Molecular Modeling

When MOLDA is running, all of the commands of MOLDA (summarized in Table 1) are allocated to the menu bar (Fig. 1). The main feature of the molecular modeling is the same as that of MOLDA4 described previously [3] except for the use of a mouse pointing device. Using the molecular modeling functions of MOLDA, the labour involved in preparing molecular structure data for molecular science is considerably reduced. Selection of a menu activates the corresponding subcommands. Menus are listed below.

1. File Menu

The ‘File’ menu deals with molecular coordinate file input and output. The valid molecule file format is MODRAST/MOLDA[3,9] and MSC’s XMol XYZ file format [10]. If no file format is specified, MODRAST/MOLDA file format is assumed by default. Molecular coordinates can be saved in VRML file format (See section 3.2.).

2. Edit Menu

The ‘Edit’ menu deals with the pasting of the Cartesian coordinates obtained from GAUSSIAN 94 or MM2. ‘Undo’ and ‘Copy’ commands are also available.
3. View Menu

The 'Edit' menu deals with the change of the screen appearance (such as showing x- and y-axes, scaling molecular size and locating the number on each atom).

Table 1. Menus/submenus and commands in MOLDA for Windows

| Menu/Submenu/Command | Description |
|----------------------|-------------|
| File                 |             |
| Open                 | Read molecular structure data in MOLDA or XMol file format |
| Save                 | Save molecular structure data in MOLDA or XMol file format |
| Save As              | Save molecular structure data in MOLDA or XMol file format as specified file name |
| Save in VRML         | Save molecular structure data in VRML file format (Dreiding sticks, ball-and-stick and spacefilling models are available) |
| Print                | Hardcopy of display |
| Exit                 | Exit MOLDA for Windows |
| Edit                 |             |
| Undo                 | Undo delete |
| Copy                 | Copy MOLDA data to clipboard |
| Paste                |             |
| MOLDA                | Paste MOLDA data in clipboard on MOLDA |
| MM2                  | Paste MM2 data in clipboard on MOLDA |
| GAUSSIAN             | Paste GAUSSIAN data in clipboard on MOLDA |
| View                 |             |
| Axes                 | Show x- and y-axes |
| Atom Number          | Locate the number on each atom |
| Auto Scaling         | Scale the size of molecule automatically |
| Cancel Atoms Automatically | Cancel duplicated atoms automatically when merged |
| Cancel Bonds Automatically | Cancel duplicated bonds automatically when merged |
| Model                |             |
| Input                |             |
| Atom                 | Input the number of atoms, the Cartesian coordinates and the atomic numbers |
| Bond                 | Generate a bond between specified two atoms |
| Alkane               | Make the all-trans conformation of an n-alkane molecule by input of the number of carbon atoms |
| Hydrogen             | Add hydrogen atoms to the carbon atoms |

http://cssjweb.chem.eng.himeji.tech.ac.jp/jcs/content.html
| Command   | Description                                                                 |
|-----------|------------------------------------------------------------------------------|
| a-No.     | Replace a specified atom by another element                                  |
| Cancel    | Delete a specified atom                                                      |
| Atom      | Delete a specified bond                                                      |
| Bond      | Delete a specified group of atoms                                            |
| Component | Place a molecule by specification of an atom so that the specified atom is at the specified position |
| Merge     | Replace an atom or a group of atoms of the molecule by another molecule      |
| Point     | Connect two molecules in such a way that their specified bonds overlap       |
| Atom      | Substitute an atom or a group of atoms with a common substituent             |
| Cn        | Do operation $C_n$                                                           |
| m         | Do operation $\sigma$                                                        |
| i         | Do operation $i$                                                             |
| Sn        | Do operation $S_n$                                                           |
| Internal Rotation | Do an internal rotation around a specified bond                             |
| Move      | Move the origin to a specified atom                                         |
| Atom      | Move the origin to the midpoint between two specified atoms                 |
| Bond      | analysis                                                                     |
| Coordinate| Give coordinates of a specified atom                                        |
| Distance  | Calculate distance between two specified atoms                              |
| Angle     | Calculate bond angle                                                         |
| Dihedral Angle | Calculate dihedral angle                                             |
| Convert   | Convert MM2 output into MOLDA data                                           |
| MM2 -> MOL| Convert AMBER trajectory file into MOLDA data as movie                      |
| AMBER -> MOL (Movie) | Convert MOLDA data into MM2 input data                                      |
| MOL -> MM2| Convert MOLDA data into GAUSSIAN 94 input data                              |
| MOL -> GAUSSIAN | Show information of this program                                           |
| Help      |                                                                              |
| Info      |                                                                              |
4. Model Menu

The 'Model' menu deals with the construction of molecular models. The input of molecular structure is commenced with the 'Input' submenu. Input data are the Cartesian coordinates of atoms, the atomic numbers and atom connection lists, which are easily generated with mouse operation. The all-trans conformation of an n-alkane molecule can be generated in a one-step operation by using the 'Alkane' command. The input structure need only be a carbon skeleton, as hydrogen atoms can be added to the skeleton by using the 'Hydrogen' command. A specified atom may be replaced by another element by using the 'a-No.' command.

The 'Merge' submenu enables any molecules made by MOLDA to be connected with each other in several modes (a specified spatial arrangement, a substitution, a ring fusion, a bridged ring-connection and a spiro ring-connection) by mouse operation.

Another interesting feature of MOLDA is the 'Group' submenu. By using the commands in the 'group' submenu, the corresponding 'symmetry operation' can be performed. The symmetry operations are defined as follows: operation 'C6z', for example, is defined so that the molecule has a $C_6$ symmetry axis around the z-axis. 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 by using this operation (Fig. 2).
5. Analysis Menu

The ‘Analysis’ menu deals with the calculation of bond distances, bond angles and dihedral angles of a molecule.

6. Convert Menu

The ‘Convert’ menu deals with the conversion of the Cartesian coordinates obtained by using several molecular science programs into MOLDA format file. The details are described in section 3.3.

3.2. The Feature of Molecular Graphics

The 3D molecular structures in VRML format can be generated by using MOLDA. These molecular structure data created by MOLDA or converted from GAUSSIAN 94, AMBER 4.0 and MM2 can be viewed in 3D by using a VRML viewer and demonstrated on WWW. At present, Dreiding-sticks (Fig. 3), spacefilling spheres (Fig. 4) and ball-and-stick models (Fig. 5) are available. The molecular models written in VRML can be easily operated by the VRML viewer not only by local users but also by remote users, who can use terminal computers connected to the Internet. Moreover, the molecular models can be viewed platform-independently, in other words, they can be displayed on the DOS/V, Macintosh and Unix machines.
Fig. 3 A Dreiding-stick model of 18-crown-6.

Fig. 4 A space-filling model of 18-crown-6.

Fig. 5 A ball-and-stick model of 18-crown-6.
3.3. The Feature of an Interface to Molecular Science Programs

When the ‘Convert’ menu is selected, the data format for MOLDA and several molecular science programs is converted to each other as described below.

1. MOLDA can make input data for molecular mechanics (MM2) or ab initio MO calculations (GAUSSIAN 94). For MM2, the conversion of data for MOLDA into those for MM2 was described in detail elsewhere [3].

2. The output files of GAUSSIAN 94, AMBER 4.0 and MM2 can be converted to the data of MOLDA format. The results of MD simulations can be animated on the screen.

4. CONCLUSION

MOLDA for Windows provides molecular graphics on the World Wide Web. The data for the molecular graphics are obtained from various programs for molecular science, such as ab initio MO, molecular dynamics and molecular mechanics calculations.

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MOLDA for Windows - パーソナルコンピュータ上での分子モデリングとVRMLを用いた分子グラフィックス

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World Wide Web (WWW)上で3次元グラフィックスを行うための新しいテクノロジーであるVirtual Reality Modeling Language (VRML)が、1995年以降、急速に発展してきた。本研究では、VRMLを分子グラフィックスの分野に応用することを目的として、1984年に開発した分子構造データ作成プログラムMOLDA4をWindows95/NTに移植すると同時に、作成された分子構造データをVRML形式のファイルに変換し、VRMLブラウザを用いて分子グラフィックスの機能を追加したMOLDA for Windowsを開発した。

http://cssjweb.chem.eng.himeji.tech.ac.jp/jcs/content.html