CyberMol – A Molecular Graphics Program System on the World Wide Web Using the Common Gateway Interface

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CyberMol, an interactive molecular graphics program system on the World Wide Web (WWW) using the Common Gateway Interface (CGI) is presented. The molecular coordinates which are inputted from the WWW browser can be transferred to the Virtual Reality Modeling Language (VRML) format file and viewed as a molecular model by using a VRML viewer on the WWW. The vibrational modes calculated by the ab initio molecular orbital program GAUSSIAN 94 can be visualized. The organic molecular structure database and the search engine for displaying molecular models by using the VRML viewer are also provided.

Keywords: Molecular graphics, World Wide Web, Common Gateway Interface, Virtual Reality Modeling Language

1. INTRODUCTION

The explosive development of the World Wide Web (WWW) has changed the computer network dramatically. Programs on the computer connected to the Internet can be easily operated by the WWW browser using the Common Gateway Interface (CGI). Furthermore, three-dimensional (3D) graphics on the Internet has recently been developed and its new technique, the Virtual Reality Modeling Language (VRML), presents the visualization of molecular models by using the VRML viewer. The 3D technique based on the VRML can be applied effectively in chemistry [1–3].

In the present work, we have developed a 3D molecular graphics program system, CyberMol, which can visualize, by using the CGI, molecular models on the WWW by the use of the VRML viewer. This system also provides the organic molecular structure database and the search engine for displaying molecular models by using the VRML viewer.

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

We use an IBM/AT compatible (DOS/V) machine, in which the Microsoft Windows NT 3.51 Workstation operating system has been installed. The EMWAC HTTP Server for Windows NT (version 0.991) program \cite{4} is used for an HTTP server. The home page of the CyberMol, whose URL is http://vb101.chem.sci.hiroshima-u.ac.jp/CyberMol1.0/, is written in the Hypertext Markup Language (HTML). A Sun workstation at the Information Processing Center of Hiroshima University is also used for executing the CGI scripts written in the Perl language. These scripts generate a VRML format text according to the corresponding inputted molecular coordinates and transport it to the HTTP server. The DOS/V machine and the Sun workstation are connected to the Internet and can be accessed to use the CyberMol. We tested the CyberMol by using a Netscape Navigator which plugged-in a Live3D as a VRML viewer.

3. OVERVIEW OF CYBERMOL AND DISCUSSION

When the home page of the CyberMol is accessed through the Internet, all of the menus are displayed on the WWW browser as shown in Fig. 1. Selection of a menu opens the corresponding page. The function and the usage of the relevant pages are given below.

![Fig. 1 The home page of the CyberMol.](image-url)
The ‘MOLDA’ page deals with the display of 3D molecular models using MOLDA format data [3,5]. The molecular coordinates and the type of molecular models (Dreiding sticks, ball-and-stick and spacefilling models are available) are inputted as shown in Fig. 2. By pushing a ‘Go!’ button, the molecular model is displayed as shown in Fig. 3.

![Fig. 2 The ‘MOLDA’ page.](image)

![Fig. 3 A Dreiding stick model of methane.](image)

The ‘Gaussian’ page deals with the display of 3D molecular models using the GAUSSIAN 94 output file [6]. The operation is the same as that of the ‘MOLDA’ page.

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XMol

The ‘XMol’ page deals with the display of 3D molecular models using XMol format data (*.xyz) [7]. The operation is the same as that of the ‘MOLDA’ page.

Vibration

The ‘Vibration’ page deals with the visualization of vibrational modes using the GAUSSIAN 94 output file. The molecular coordinates and the displacements of atoms calculated by the GAUSSIAN 94 program are inputted as shown in Fig. 4. By pushing a ‘Go!’ button, the vibrational mode is displayed as shown in Fig. 5.

![Fig. 4 The ‘Vibration’ page.](image-url)
Search

The ‘Search’ page deals with the search of molecular coordinates from the organic molecular structure database provided by Nagao [8]. To search for the molecular structure data, enter a keyword (a Perl regular expression is also available). After searching, the ball-and-stick model of the molecule is displayed on the VRML viewer.

Link

The ‘Link’ page deals with the links to other VRML chemistry resources.

Help

The ‘Help’ page deals with the help for using the CyberMol.

By using these functions, the CyberMol can be easily operated by the WWW browser using the CGI not only by local users but also by remote users who can use terminal computers which are connected to the Internet. Moreover, the system is used platform-independently; in other words, the molecular models can be displayed on the DOS/V, Macintosh and Unix machines by using the CyberMol. For a long time, computer software has been dependent on hardware and operating systems. On the contrary, the present system provides a new programming paradigm that software should work platform-independently. The new programming approach will change the programming styles in computer chemistry.

4. CONCLUSION

CyberMol provides molecular graphics on the WWW by using the MOLDA, XMol and GAUSSIAN 94 format data. The organic molecular structure database and the search engine for displaying molecular models by using the VRML viewer are useful in chemical education. The system can be easily operated by the WWW browser using the

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CGI not only by local users but also by remote users who can use terminal computers which are connected to the Internet. In the next stage, the CyberMol will offer the function of the molecular modeling and control the ab initio molecular orbital calculation and molecular dynamics simulation programs by the combined use of the CGI, VRML and Java technologies. This forthcoming system will generate the new age of molecular science and molecular technology.

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CyberMol – CGI 機能を用いた World Wide Web 上での分子グラフィックスシステム

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World Wide Web (WWW)上で機種に依存しない分子模型の3次元表示を可能とするために, Virtual Reality Modeling Language (VRML)とCommon Gateway Interface (CGI)を併用した分子グラフィックスシステムを開発した。このシステムでは, WWWブラウザから分子の直交座標値を入力することにより, その模型図をインターネットに接続されている端末のディスプレイに表示することが可能である。また, 非経験的分子軌道計算プログラムGAUSSIAN94により得られた分子の振動形の表示機能や有機化合物分子座標データ集の検索機能ももつ。

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