3D Molecular Graphics on the World Wide Web

H. Vollhardt[1)] and J. Brickmann[1,2,*)]

[1)] Institut für Physikalische Chemie and
[2)] Darmstädter Zentrum für wissenschaftliches Rechnen
Technische Hochschule Darmstadt
Petersenstr. 20, D-64287 Darmstadt, Germany

Abstract
The Virtual Reality Modeling Language (VRML) is a new tool for the information transfer on the World Wide Web (WWW). We present a short description and some applications in the field of molecular graphics of this new, object oriented language. It is shown that the usage of VRML is a very efficient and powerful method for the transport of molecular models over the net.

1 Introduction

The development of the World Wide Web (WWW) in 1989 has changed the internet capacity dramatically. Before the introduction of the WWW, data have been exchanged only within small groups. With the WWW, it is possible to provide information in various forms for the whole internet community. With hyperlinks, every information can be referenced from anywhere on the internet. The WWW has turned the entire internet into one large storage for information of any kind.

The new information exchange technology has already lead to a rapid growth of electronic publishing media. The electronic journals have extended the traditional form of presentations mainly composed of text and illustrations. However, none of the new media types, such as audio or animation sequences, are appropriate for the representation of 3D scenarios. The formats used for images and animations are of pixel based nature and therefore fixed in size and rigid in their behavior. The viewers are not able to change the point of view with respect to the object shown. In order to get a 3D impression of an object, at least two images are needed and the point of view is still preselected by the producer of the scenario. In molecular science 3D impressions are absolutely neccessary in order to transfer and understand complex structural information. Traditionally, the structural information is transfered via standard file formats (e.g., Brookhaven Protein Data Bank, PDB) containing atom types and 3D coordinates. The

[*] Author to whom all correspondence should be addressed

visualization and manipulation is done locally with the aid of modeling software packages. There was no way up to now to transfer the 3D scenario directly. This gap can be filled using the Virtual Reality Modeling Language (VRML)[1].

2 Short description of VRML

The idea for VRML was born in 1994 at the first WWW conference in Geneva. A group of attendees agreed on the need for a common language to specify 3D-scene description and WWW hyperlinks. Immediately after the conference, the 'www-vrml' mailing list[2] was established starting the discussion on the developement of a language specification. The list members agreed to adapt VRML from a subset of the Open Inventor ASCII File Format[3] from Silicon Graphics, Inc. In the present version 1.0 specification of VRML, this subset was extended with networking capabilities, such as WWW hyperlinks. With this feature, VRML is an equivalent to the hypertext markup language (HTML)[4]. Like HTML files describe the layout of 2D-text pages to be displayed by WWW browsers, VRML files describe the layout of 3D scenarios. The structure of the language can be characterized as follows.

2.1 Nodes

A VRML file describes a scene in an object oriented manner. The basic elements building the objects are called *nodes*. The nodes can be devided into five different categories:

(i) *Shape nodes*
represent 3D geometry objects, such as points, lines, polygons, or even more complex shapes like cubes, spheres, cones, or cylinders. They are the only nodes which are visible.

(ii) *Property nodes*
affect the appearance and the characteristics of the other nodes. They can be divided into three subgroups.
   (a) *Transform nodes* perform coordinate transformations on the given geometry (e.g., rotation, translation, scale, etc.).
   (b) *Appearance nodes* affect an object's appearance, such as color, material properties, or texture maps.
   (c) *Metrics nodes* contain coordinates, normals, texture coordinates, and other geometric information.

(iii) *Group nodes* are used to collect nodes to implement a hierachical structure. Some of them can isolate the effects of their children from the rest of the scene.

(iv) *Light nodes*
are used to define different types of light sources to illuminate the scene (e.g., point lights or spot lights).

(v) *Camera nodes*
are used to define different points of view, for example to create a guided tour through the virtual scenario.

Nodes have some further characteristics. They have associated *fields* describing their parameters (e.g., the height of a cone, the position of a light source, etc). A *name* can be assigned to a node, which allows to use it later everywhere in the scene. This mechanism, called *instancing*, reduces the neccessary memory capacity because only one copy of the node is allocated and it can be referenced multiple times (see Figure 1 for definition of the oxygen atoms).

The nodes (i)-(v) represent a subset of Open Inventor[3]. Extensions have been neccessary in order to establish a communication capacity of the language. Two new kinds of nodes have been introduced:

(i) The *WWWInline* node is used to load additional VRML files from elsewhere on the WWW into the scene. This is accomplished with a field, that defines a Uniform Resource Locator (URL)[5], i.e., the location on the internet where the object is stored. With this feature, large and complex scenes can be composed from a library of smaller objects.

(ii) The *WWWAnchor* node is the equivalent to the anchor tag in HTML. Hence, it represents the WWW hyperlink. Because this node is a group node, all its children act as one hyperlink.

The VRML specification supports the extension of the node set. Node types not defined in standard VRML are introduced by *self-describing* nodes. These nodes have to hold a description of all their fields.

Molecular Inventor[6], developed by Silicon Graphics, is an extension of the Open Inventor base class set. Thus, it can also be used to extend the VRML node set. Molecular Inventor provides new types of nodes for molecular graphics rendering primitives like high-quality lines, stereo in a window, fast construction of isosurfaces and molecular surfaces, volume rendering, slice planes, property mapping, etc. The node set can be used to store the complete information about a given molecule which can be exchanged locally between applications or globally via the WWW.

2.2 Scene Graph

In order to describe a 3D scenario, the nodes building the contents have to be arranged in a hierachical structure called 'scene graph'. A scene graph defines the ordering of the nodes and therefore the layout of the 3D scenario. The ordering is important because nodes earlier in the scene can affect nodes coming up later. Figure 1 shows an example of a scene graph for a carbon dioxid molecule in CPK representation. Everytime the molecular model has to be rendered, this scene graph is traversed from top to bottom and from left to right.

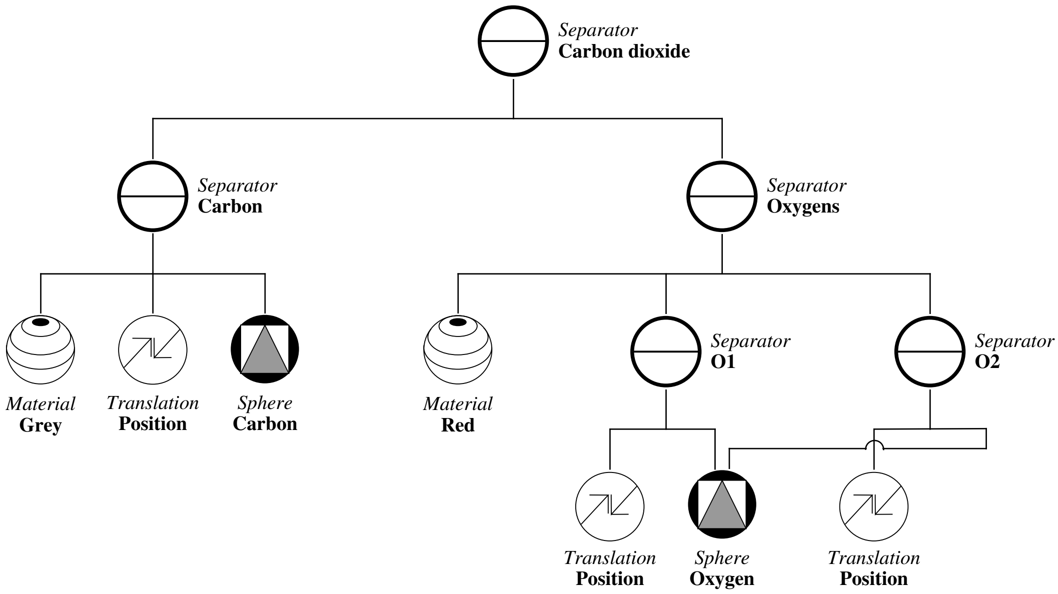

Figure 1: Scene graph of a carbon dioxid molecule (CPK model). The different symbols represent the different types of nodes. The definition of the two oxygen atoms is an example how one instance of a node can be referenced multiple times.

Table 1: Comparison of file formats.

Format	GIF image	MPEG stream	VRML scene
resolution [pixel x pixel]	640 x 480	320 x 256	$\infty^{*)}$
colors	256	256	$\infty^{*)}$
frames	1	90	∞
file size [KB]	27	170	14
compressed (gzip) [KB]	27	170	3

$^{*)}$ the final output depends on the graphics hardware

3 VRML in comparison with other file formats

The currently used file formats for the transfer of nontextual information are sometimes ineffective. The usage of image formats like GIF[7] or JFIF[8] for molecular structures is insufficient. Because of their 2D nature, single pictures or sequences of pictures are a very poor medium to store and transfer 3D molecular information. Therefore, small animation sequences are often used to cause a better 3D impression by changing the point of view continiously. But both media are fixed in size and resolution. Whereas, objects in VRML files are stored based on their 3D coordinates. Thus, VRML scenes are in principle infinitely scalable. This is demonstrated in Table 1 comparing some properties of files depicting the same object in different formats. The corresponding molecular model is shown in Figure 2. Because, VRML files are written in ASCII format, they can be ideally compressed. This again reduces the transmission times over the internet.

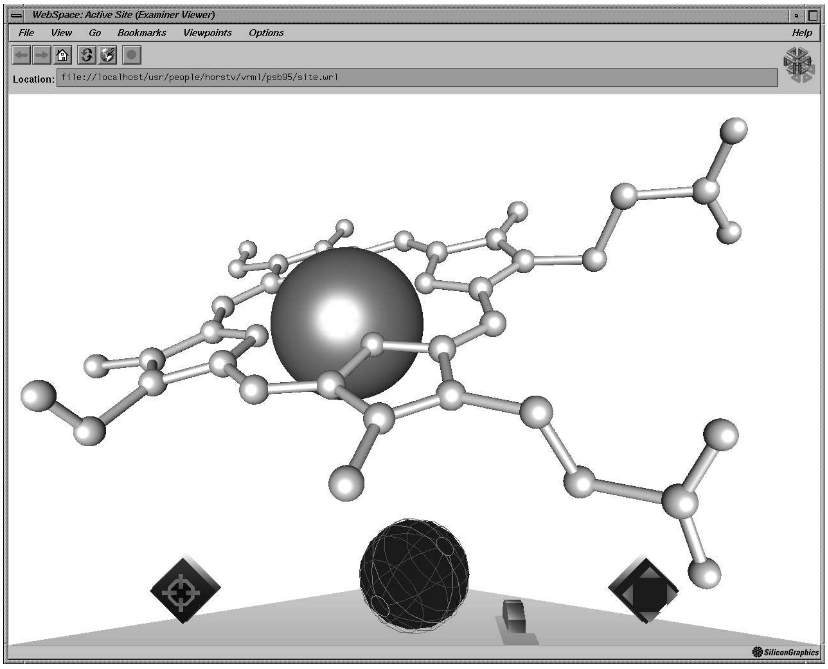

Figure 2: Active site of the P450 enzymes, a porphyrine molecule with a central iron atom shown in ball-and-stick representation. The navigation tools of the VRML viewer *WebSpace* are located at the bottom.

The development of chemical MIME[9] (Multipurpose Internet Mail Extensions) types[10] has lead to a different approach for the transport of chemical information. MIME types are used to specify the contents of a given file transfered by the WWW (e.g., PDB file, GAUSSIAN output, MOPAC output, etc.). This method extends the possibilities of chemical information transfer, but has also some disadvantages. Various applications with different user interfaces have to be installed and configured, because of the different file formats. The author of the information has no control how the reader is using and filtering the data. With VRML, the author controls the layout of the final output and the reader has to learn only one user interface. Additionally, with hyperlinks, the author can add annotations to the objects describing them in various forms, like text, audio, or video.

4 Example: The VRML pages of the authors institution

Some of the capabilities of VRML are demonstrated at the VRML page[11] of the WWW server at the Institute of Physical Chemistry, TH Darmstadt with examples from protein research, visualization of molecular structures and atomic orbitals.

4.1 The cytochrome P450 receptor modelled with static VRML files

Cytochrome P450 enzymes play a central role in carcinogenesis and toxicology. Substrates, like nitrosamines, were activated after passing a kind of channel[12] at the porphyrine binding site located at the center of the enzyme (Figure 3). We use a widely accepted model for the P450 enzymes based on the crystal structure of cytochrome P450cam[13].

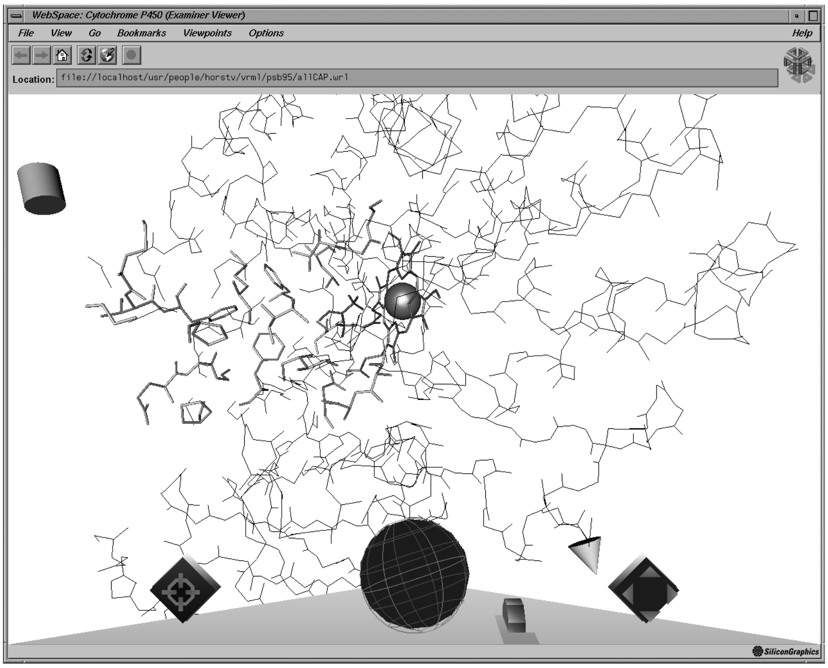

Figure 3: Wireframe model of cytochrome P450cam. The channel residues and the active site at the center are slightly darker. The model is surrounded by hyperlinks represented as cones and cylinders.

We have devided the VRML model of P450 into four parts, protein backbone, channel residues, active site and substrate. These parts are stored in separate files. To reconstruct the complete enzyme model all files can be combined using the WWWInline node. Additionally, each node acts as a hyperlink pointing to the VRML file of the isolated part allowing the user to "zoom" into the details of the model. Because, one hyperlink can reference only one URL, we have added 3D buttons (represented by smaller objects around the model scenarios) acting as additional hyperlinks. Some of them can be used to switch between different representations (wireframe, ball-and-stick, CPK model, etc.). Others are linked to textual information about the given object. In this way, it is easy to navigate through the different components of the enzyme and obtain related data.

The wireframe models are build of line nodes in combination with a set of all coordinates. The ball-and-stick and CPK models are made of the more complex shape nodes. All basic elements of a molecular structure are modelled with one single VRML node. Each atom is represented by one sphere and each bond is made of one cylinder. Only bonds between atoms of different color are build of two cylinders. Because every shape node has a default position and orientation, we have placed a matrix transfromation ahead of each shape and put both nodes inside a separator to isolate their effects. As a result, the VRML files are rather small (see Table 1).

VRML can be used for building user-defined shapes using polygon nodes. We have demonstrated this with the solvent accessible surface[14] of the channel region (Figure 4). These surfaces can be color-coded with molecular properties (e.g., hydrophobicity). This can be achieved using gouraud shading[15] or texture mapping[16] techniques.

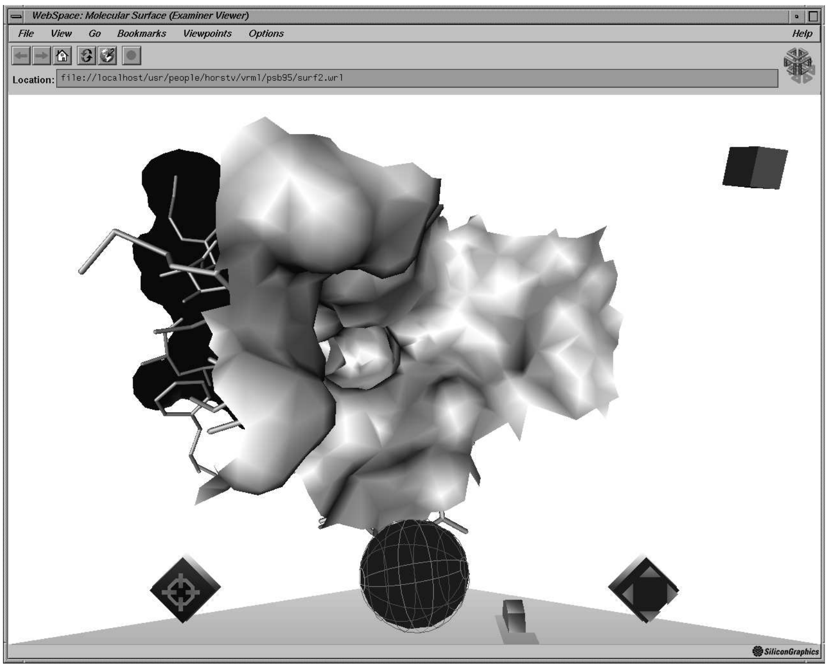

Figure 4: The solvent accessible surface of the substrate channel. The channel residues are represented by a stick model.

4.2 Interactively created VRML files

VRML cannot only be used in order to describe static scenarios. The HTTP (HyperText Transfer Protocol)[17] provides a second, powerful mechanism for the transfer of data over the WWW. Instead of sending prebuild files, the data can be generated interactively with CGI[18] (Common Gateway Interface) scripts. The output of these scripts can be controlled with parameters, which again can be set by the user through forms. We will demonstrate the flexibility of this interface, provided by most of the WWW browsers with several examples.

4.2.1 User-controlled models of P450[19]

All amino acids of the P450 backbone have been modelled separately and stored as individual VRML files building a small database. The user selects amino acids from this database, which then are combined to a individual model of cytochrome P450. Additionally, the user can chose the representation and whether the active site should be included or not.

4.2.2 Visualization of molecular structures[20]

An interface to a small database of molecular structures, stored in the PDB file format was constructed. The form permits the user to select one of the molecules from the database and the representation (e.g., wireframe, ball-and-stick, etc.) as well as the color. After sending the request to the WWW server, the user receives the VRML file, generated from the PDB file, within a few seconds.

4.2.3 Visualization of distributed databases[21]

We have extended the concept of visualization of local databases (local relativ to the WWW server). This example shows how molecular structures stored in a database anywhere on the internet can be visualized. Again, the user selects the representation of the final output, but additionally a URL is given. Before the server sends the VRML file back to the client, he loads the dataset from the given URL. This methods has three handicaps up to now.

(i) The total operation may take twice as long as in the previous example and
(ii) the client does not receive any notification about the first step (the loading of the molecular structure).
(iii) Only those database formats can be treated properly which are known to the server.

4.2.4 Visualization of atomic orbitals[22]

The previous three examples demonstrated the visualization of molecular scenarios based on information from existing databases. The final one shows how VRML can be used to visualize virtual scenes which are defined on the basis of analytical expressions and algorithms. The atomic orbitals of the hydrogen atom are taken as examples. The visualization of the electronic wavefunctions is based on the representation of isocontour surfaces (Figure 5). The procedure has four steps. The user selects the orbital type (e.g., 1s, $2p_x$, etc.). The corresponding wavefunction is calculated at points of a 3D grid. The size of the grid and the spacing of the grid points can be selected as well. In the second step a isocontour surface with the user-defined contour value is generated using a marching cube algorithm[23]. Within the third step the surface is converted into a VRML file. The user can chose the type of representation (dots, wireframe, or solid). Finally, the VRML file can be compressed by a factor between 4 and 5 before it is returned to the user. All steps together require only a few seconds on a standard workstation.

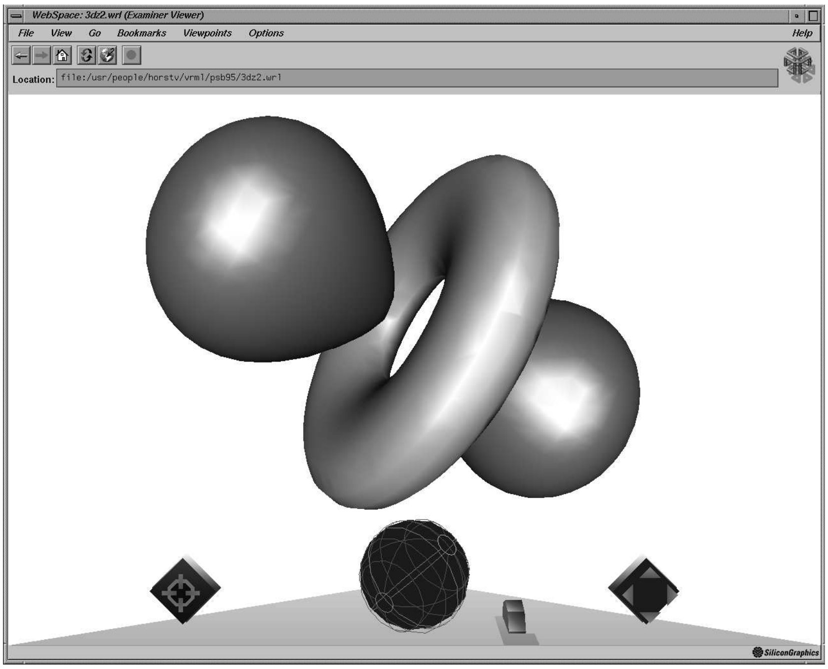

Figure 5: Two isocontour surfaces of the $3d_{z2}$ orbital.

5 Conclusions and Outlook

The rapid, nearly exploding growth of the WWW community has already demonstrated how powerful this new communication concept is. We predict a similar growth in the field of VRML, at least in areas where 3D visualization is of particular importance. Because VRML is an equivalent to HTML, it is more than a simple file format for the storage of data, like GIF or MPEG. With the WWW hyperlinks information can be referenced from elsewhere on the internet. In the current state the VRML browsers can be used as platform-independent frontends for database and computational servers.

The implementation of *dynamic behavior* and *interactivity* is one of the next steps in the development of the VRML specification. With this set of features

VRML could become a standard data-exchange format for collaborative applications.

6 Acknowledgements

We like to thank H. Look, Silicon Graphics, Inc. for providing the early versions of the VRML viewer, WebSpace[24]. This work is partly supported by the Fonds der chemischen Industrie, Frankfurt.

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