ACD/3D Viewer

Version 11.0 for Microsoft Windows

User's Guide

Viewing 3D Structures and Calculating their Structural Parameters

Advanced Chemistry Development, Inc.

Table of Contents

Before You Begin

Thank you for purchasing ACD/3D Viewer. We have endeavored to produce the easiest to use 3D chemical display program available today.

About This Guide

Completion of this guide should give you the tools needed to get started with ACD/3D Viewer, it is designed for either online use or to be printed and used as a "hard copy" version.

The screen shots shown throughout this reference manual have been taken with a relatively small window size.

The colors and other properties of the window elements described throughout this manual correspond with the default Windows Display Properties.

This guide is provided in electronic form, readable with Adobe Acrobat software. If you cannot locate an index topic you need please do a text string search for the relevant word or phrase, or related words.

Advanced Understanding

This guide is intended to be a part of the technical documentation for ACD/Labs software. To study ACD/Labs products gradually, we recommend the following order of working through the technical documentation:

Documents for ACD/ChemSketch and ACD/Dictionary familiarize you with features of drawing and looking up structures.

ACD/Forms Manager is required to learn how to create input dialog boxes for user data and an interface for consistent database input.

Mouse Conventions

You may perform several actions during your work with this software; the following specific words are used to describe them:

- *Point to* means move the mouse pointer ⭰ to an item.
- *Click* or left-click means point to an item, and press the left mouse button.
- *Right-click* means point to an item, and press the right mouse button.
- *Double-click* means point to an item, and quickly press the left mouse button twice.
- *Drag* means point to an item, press and hold down the left mouse button while you move the item.

- **Select** means highlight or make an interface element active by either clicking it or dragging over it (other actions are possible if specified in documentation). If used in "select the check box", it means that the check box should be marked with a tick (as opposed to "clear the check box" when the check box should be cleared, without a mark).

For More Information…

To see the latest in ACD/Labs software and services, please visit our Web site at

http://www.acdlabs.com

Our Web site is being accessed at the rate of tens of thousands of "hits" per day. There's a reason for this: much is offered through our Web site. As of Autumn 2006, we offer free ChemSketch 10.0, an ACD/Log*P* Freeware Add-on for ChemSketch, a free ISIS 3D Add-in, free ChemDraw extensions, and a free 2-week demo key for "Interactive Laboratory" sessions where you can run test calculations using Java applets without purchasing software. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ChemSketch) available for download.

We are constantly updating the information on our Web site. The Web site will tell you at which scientific conferences you can visit the ACD/Labs booth. You can browse the Frequently Asked Questions page or drop in and "chat" on our newsgroup, which can also be reached via our web page.

If you would like to stay informed of the latest developments in chemical software at ACD/Labs, please be sure to sign up for e-mail broadcasts at our Web site page:

http://www.acdlabs.com/feedback/mailing.html

If you would like to participate in the ACD/Labs forums, please access:

http://forum.acdlabs.com

How to Contact Us

We are accessible through our Web site, phone, fax, and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability, and general issues should be directed to:

info@acdlabs.com

Technical and scientific support issues should be addressed by visiting:

http://support.acdlabs.com

Please tell us the name of the software purchaser; the product name, version number, build number, and license ID of the product you are contacting us about (from the **Help** menu, choose **About** to find this information); as well as a description of the problem you are having. If applicable, please tell us the name of the distributor from whom you purchased the software.

Online Updates

All PC-based ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. The updates are small fixes, for example, bringing the actual version number of a program from 11.00 to 11.01. Please refer to the document, "Online Updates," included with the rest of the product documentation in your Documents folder for more information on this, or contact our technical support department.

1. Introduction

1.1 What is ACD/3D Viewer?

ACD/3D Viewer is a fast yet accurate 3D modeling and visualization program. It is fully integrated with ACD/ChemSketch, allowing you to draw 2D structures and quickly obtain their 3D representations in a striking color display. With ACD/3D Viewer you can:

- Manipulate 3D models: move, 2D and 3D rotate, resize, change styles, and colors;
- Display a 3-D structure as stick, ball-and-stick, spheres, or disks;
- Add an overlay of small-dots at approximately the Van der Waals radius level to the solid 3-D structure;
- Measure and change bond lengths, plane bond angles, and torsion angles;
- Optimize the structure using a 3-D CHARMM-type of force field;
- Switch from 3D to 2D display in the ChemSketch window at the click of a button;
- Set the 3D molecule to Auto-rotate, with or without changing the style of structure display;
- Rotate and move selected atoms rather than entire structures;
- Change and delete atoms, assign the center of rotation to an atom;
- Create movies and save them as .GIF files;
- View 3D structure in perspective; and
- Export 3D models to other geometry optimization programs and use them as good starting configurations.

1.2 3D Optimization Algorithm

The 3D optimization algorithm rapidly transforms the planar (2D) structure from ChemSketch into a realistic 3-dimensional structure. It is based on modified molecular mechanics which take into account bond stretching, angle bending, internal rotation, and Van der Waals non-bonded interactions. Modifications include minor simplification of potential functions and enforcement of the minimization scheme by additional heuristic algorithms for dealing with "bad" starting conformations.

The 3D optimization algorithm is a proprietary version of molecular mechanics with the force field initially based on CHARMM parametrization.[1] The modifications involve some simplification and were intended to increase the stability and speed of computation. Note that 3D-optimizer is NOT a full-scale molecular mechanics engine. Its design aims to reliably reproduce reasonable conformations from (possibly very unreasonable) 2D drawings, rather than to precisely optimize 3D structures.

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[1] Refer to B.R. Brooks, R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan, and M. Karplus. CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. *J. Comput. Chem.* 4 187–217 (1983).

Occasionally the 3D optimization produces a molecular conformation different from what you expect. It is the very essence of the conformational analysis that molecules typically have many possible conformations. The optimizer finds only one, and it is not necessarily the one you have expected. For example, you probably expect a cyclohexane fragment to be a chair, but the optimizer may generate a twist-boat, which is also one of its suitable conformations (indeed, in many structures this fragment exists in a twisted form). To obtain another conformation, move some atoms in the resultant 3D structure to make the initial structure closer to the final conformation, and then optimize the structure once again.

If you try to obtain a specific enantiomer for a structure with chiral centers, in the process of optimization, the configuration input may occasionally change to an opposite one. To solve the problem, it is usually enough to draw all four substituents of the chiral carbon atom and use both **Up** and **Down Stereo Bond** tools to define the required direction of bonds in the initial 2D structure. If it doesn't work, you can move the atoms manually in the resulted 3D structure and optimize the structure once again. In any case, we recommend answering "No" when you are asked whether to remove hydrogens before starting optimization in the unfolding **3D Structure Optimization** dialog box.

1.2.1 Limitations of ACD/3D Optimizer

ACD/3D Viewer can only optimize structures containing atoms from Hydrogen to Xenon with standard valence and bonding states. Also, it does not take into account hydrogen bonding.

The maximum allowed number of atoms in the structure to be optimized is 250 including implicit hydrogen atoms.

2. Basics of ACD/3D Viewer

2.1 Objectives

This chapter will familiarize you with:

- Starting the program;
- Setting and changing file associations;
- Changing default directories for opening and saving files; and
- Exiting the program.

Instructions for system requirements, and for installing and uninstalling the software are provided on a separate sheet of paper, shipped with the software itself.

2.2 Starting ACD/3D Viewer

Once ACD/3D Viewer has been installed on your computer, follow these basic steps to start it:

1. Start Microsoft Windows.

2. Double-click the 3D Viewer icon.
   –OR–
   On the **Start** menu, point to **ACD/Labs**, and then choose the 3D Viewer icon.
   –OR–
   Double-click the program file SHOW3D.EXE in the folder where you have installed all ACD/Labs software. By default this is ACD11.
   –OR–
   If you have other ACD/Labs programs running, from the **ACD/Labs** menu, choose **3D Viewer**.

   You should see an opening splash screen. If this is the freeware version, you will see a 15-second list of ACD/Labs products scroll by. Be patient and click **Cancel** when it becomes active.

2.3 Setting File Associations

If this is the first time you have started the program, the **File Associations** dialog box will appear.

> **Note**   If you open the **File Associations** dialog box (from the **File** menu, choose **File Associations**) under Windows NT but have no rights to change file associations, a warning message appears. Contact your system administrator to resolve this matter.

This contains a selectable list of file extensions and file types which you may want to open automatically with ACD/Labs software from now on. If so, click the check boxes of the file formats you want to add, and then click **Yes**.

If you do not want to have 3D Viewer automatically open files with the listed extension, or are not sure, leave the check boxes blank and click **No**.

2.3.1 Changing File Associations

If you have not selected all formats, the default file association can be viewed or changed at any time; from the **File** menu, choose **File Associations**. If you have selected all formats, then you receive a message, "all supported file types are already associated with the current application". In this case, you can change the file associations through Windows Explorer.

1. Open Windows Explorer, and select a file with the extension for which you want to create the association.
2. Hold down SHIFT and right-click the file. From the shortcut menu, choose **Open With**.
3. Set the application that should be used to open the file and select the **Always use this program** check box.
4. Click **OK** and close Windows Explorer.

2.4 Changing Default Directories

If you are running a single-user (stand-alone) copy of ACD/3D Viewer, the default directory settings are likely fine.

If you have a network copy, it is advisable to change the default directory settings in the ACD/Labs software so that the default drive for saving work-in-progress is the user's local hard drive, not the remote server. After creating local access for either limited or unlimited numbers of seats, then at each local installation:

1. In the ChemSketch window, from the **Options** menu, choose **Preferences**.
2. Click the **General** tab. In the **Default** box, specify the directory that will be opened every time you open the **Import**, **Open**, **Save**, or **Export** dialog boxes in the ChemSketch window:

> **Note** In the Private box you can set the directory for recording the configuration of the ChemSketch program (e.g., TEMPLATE.CFG and GRSTYLES.STL files).

3. Click **OK**.

4. Switch to the 3D window, from the **Options** menu, choose **Set Default Folder** and specify the required folder for opening and saving files. Click **OK**.

2.5 Exiting ACD/3D Viewer

You can exit from the program in any of the following ways:

- In the upper right-hand corner of the title bar of any window, click ⊠.

  –OR–

- From the **ACD/Labs** menu, choose **Close All**. This will attempt to close all ACD/Labs programs that are currently open, one right after the next.

  –OR–

- From the **File** menu, choose **Exit**. This will close only the currently open ACD/Labs program.

You will be prompted to save your work in the appropriate file formats, depending on the window that you are exiting.

3. Operating with Molecules View

3.1 Objectives

In this chapter you will learn how to:

- Insert molecules into the 3D window and carry out 3D optimization;

- Customize the view of the molecules (position, size, color, atom radii);

- Save and load view settings; and

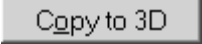- Measure and change the distance between atoms, and calculate and change the angle between bonds.

## 3.2 Inserting a Molecule and 3D Optimizing

1. Start ACD/3D Viewer as described above.

2. On the Window Switching bar, click **ChemSketch** `ChemSketch` . This will switch you to the ChemSketch window.

3. In the upper right part of the window, click **Dictionary** .

   > **Note** The ChemSketch Freeware version does not include the Dictionary module. This module is only available with the commercial version of ChemSketch. If you are using the ChemSketch Freeware version, draw any desired structure using the ChemSketch interface tools. (For details on drawing structures, refer to the *ACD/ChemSketch Tutorial.*)

4. In the **Quick Search** box of the **ACD/Dictionary** dialog box that appears, type a few keystrokes for the name "*cinchonidine*". (Cinchonidine is an anti-malarial agent that is extracted from the bark of various species of Cinchona.)

5. As soon as the required name is selected in the list and the corresponding structure is displayed, click **OK**. Note that the shadow of the selected structure hangs over the cursor. Click the workspace to place the structure in the ChemSketch window:
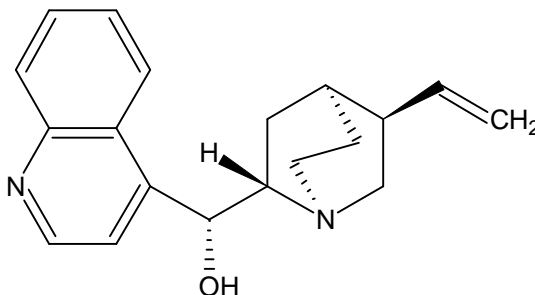
6. On the Window Switching bar, click **Copy to 3D** [Copy to 3D] to transfer the molecule into the ACD/3D Viewer interface. You will see a simple stick figure appear in the 3D window:
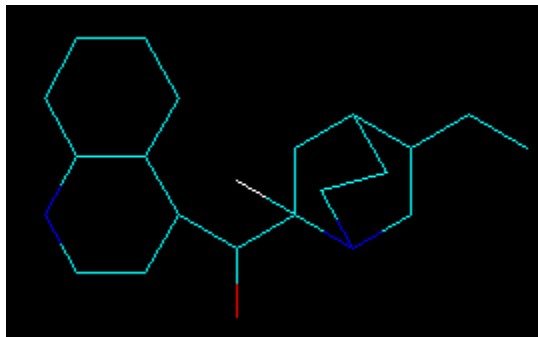

7. To create a 3D model of a 2D chemical structure, click **3D Optimization** [icon]. Note that the hydrogens are added:
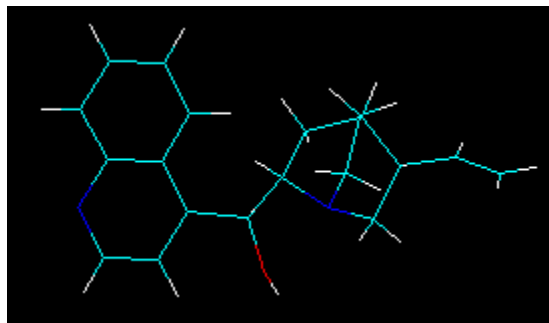
3.3 Customizing Molecule View

3.3.1 Changing Structure Representation

1. To represent the current structure as balls and sticks, click **Balls and Sticks** .

2. To add a dots halo to the current molecule view, click **With Dots** . The structure will look something like this:
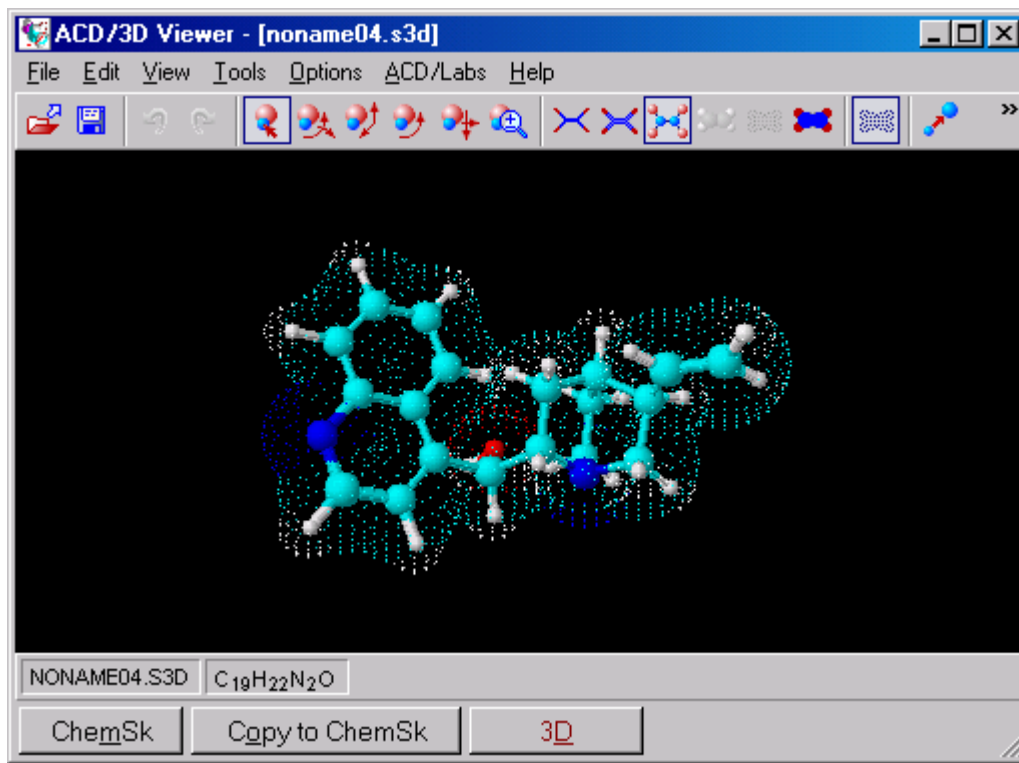
3. To display multiple bonds, switch to the Wireframe mode by clicking on the Top toolbar, and then from the **View** menu, choose **Show Multiple Bonds**:
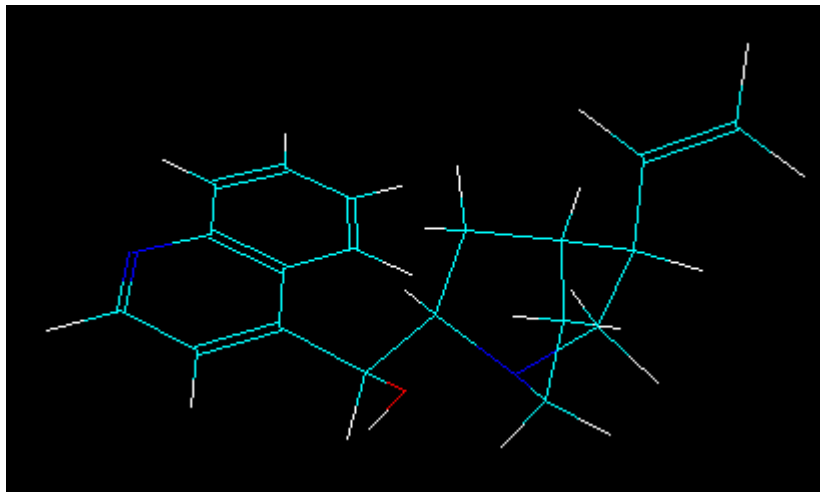
3.3.2 Labeling Atoms

3D Viewer allows you to display the periodic name of a single atom or of all atoms at once.

1. Right-click the atom you want to label.

2. In the shortcut menu, choose **Label Atom**. The label is immediately displayed:

> **Tip** To adjust the font used for the labels, from the **Options** menu, choose **Labels Font**.
> To adjust the size of the labels in the zooming mode, from the **Options** menu, choose
> **Scale Labels**.

3. To label each atom in the 3D Viewer window, from the **View** menu, choose **Label All**.

4. For the present, we do not need the labels, so you may hide them by choosing **Label None**
   from the **View** menu.

3.3.3 Displaying Atom Information

For convenience purposes, you can set up 3D Viewer so that it displays hints containing data on
each atom. The data includes the atom name, number, and its coordinates. The name and
number of an atom is displayed on a hint that appears as you point to the atom:


The coordinates can be seen on the status bar:

All of these parameters are displayed by default. So, you just need to make sure everything is
okay since we will need these hints later on in this guide. To adjust the settings, from the
Options menu, choose **Atom Information** and ensure all check boxes are selected in the **Atom
Information** dialog box:
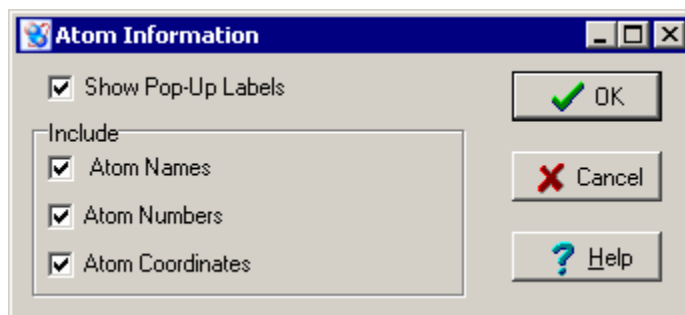
3.3.4 Rotating, Moving and Zooming

ACD/3D Viewer gives you a wide range of tools for moving and rotating molecules or separate atoms both manually and automatically.

1. Practice manual rotation; from the **Tools** menu, choose **Z-rotate Mode** or **Rotate Mode** or click **Rotate** [icon] or **3D Rotate** [icon] respectively, and then drag in the workspace to rotate in the 2 or 3 dimensions system respectively.

2. To resize the structure display, from the **Tools** menu, choose **Zoom Mode** or click **Resize** [icon], and then drag. Dragging from the center of the structure to the border of the screen makes the structure larger and dragging to the center of the structure makes it smaller.

3. Now, let us turn the molecule around the Y axis at the angle of 120 degrees. To set the axis and angle, from the **Options** menu, choose **Fixed Angle Rotation Setup**.

4. In the **Fixed Angle Rotation Setup** dialog box, in the **Rotation Axis** area, select **Y axis** and in the **Rotation Angle** box, type *120*:
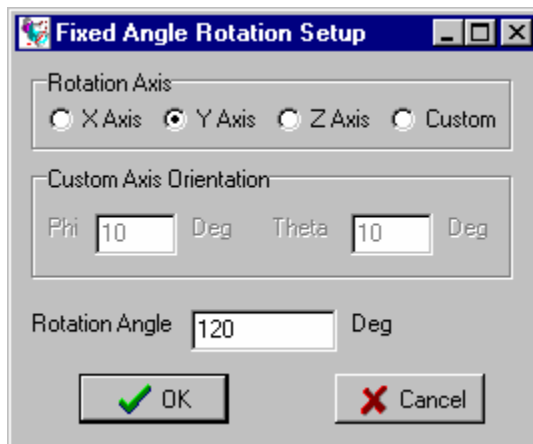
5. From the **Tools** menu, choose **Fixed Angle Rotation Mode** or, on the Top toolbar, click **Fixed Angle Rotation** [icon]. Each click in the workspace will rotate the molecule about the Y axis at the set rotation angle. Click as many times as required until you get a clear view of the molecule:
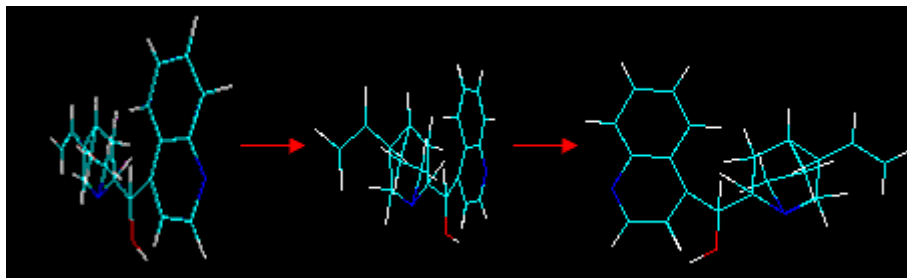
6. 3D Viewer also allows you to rotate a molecule around a selected atom. Right-click C#10:
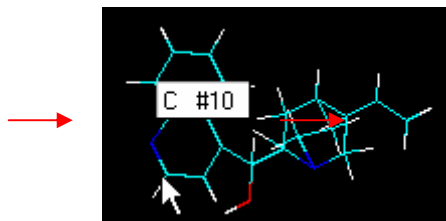
7. In the shortcut menu, choose **Center on Atom**. The molecule is automatically relocated so that the C#10 atom is in the center of the workspace.

8. From the **Tools** menu, choose **Auto Rotate** or **Auto Rotate and Change Style**. Both of these commands rotate the molecules automatically, however, unlike the former, the latter also changes the representation style of the molecules being rotated.

> **Tip** There may be cases when you need to rotate a part of a molecule rather than the entire molecule or when you have several molecules in the workspace and want to rotate or move one of these. In both cases you should select the appropriate atoms one by one (on the Top toolbar, click **Select Atoms** , and then click the appropriate atoms). To rotate or move the selected atoms only, from the **Edit** menu, choose **Manipulate Selected**, and then apply any manual or automatic rotation or movement mode.

3.3.5 Changing Colors

1. From the **Options** menu, choose **Colors** or click **Set Colors** to display the **Colors** dialog box:
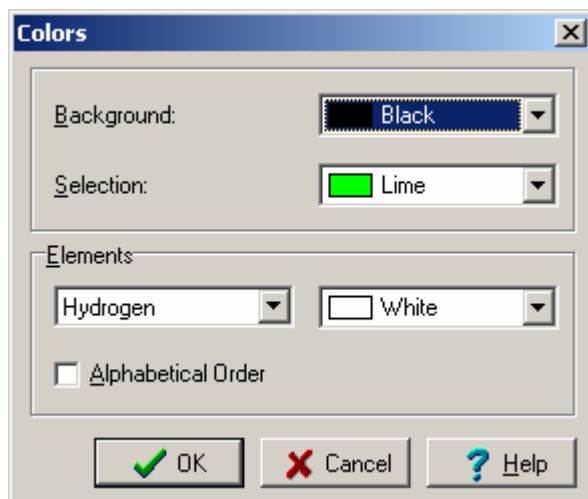
2. To change the color of the background of the display, select the desired color in the **Background** list.

> **Tip** If you are printing a lot, it is best to change the background to white to save toner.

3. The selected atoms are given a special highlight color. The default is lime. To change the color of the atoms that are selected, from the **Selection** list, choose the desired color.

4. To change the color of a chemical element, in the **Elements** area, click the name of the element in the list and then choose the desired color to the right.

> **Note** Selecting the **Alphabetical Order** check box sorts the names of the elements in the list; otherwise, the elements are listed in the order they appear in the Periodic Table of Elements.

3.3.6 Obtaining the Mirror View

1. Click **Mirror** [icon] to obtain a mirror image of the currently displayed structure. All the stereo centers present in the initial structure will be inverted in this case.
2. To return back to the initial view, click this button again.

3.3.7 Inverting Structure Center

1. Click **Invert Center** [icon], and then click the atom to invert. This tool inverts the configuration of chiral center by changing the spatial position of one or several substituents of the selected atom.

   > **Note**   After the current operation it may be necessary to optimize the chemical structure once more. To perform this, on the Top toolbar, click **3D Optimization** [icon].

2. To return back to the initial structure view, click **Invert Center** [icon] again.

3.3.8 Changing Atom Radius of a Specific Element

1. From the **Options** menu, choose **Radii** to open the **Atomic Radii** dialog box containing the default settings for atom radii of various elements:
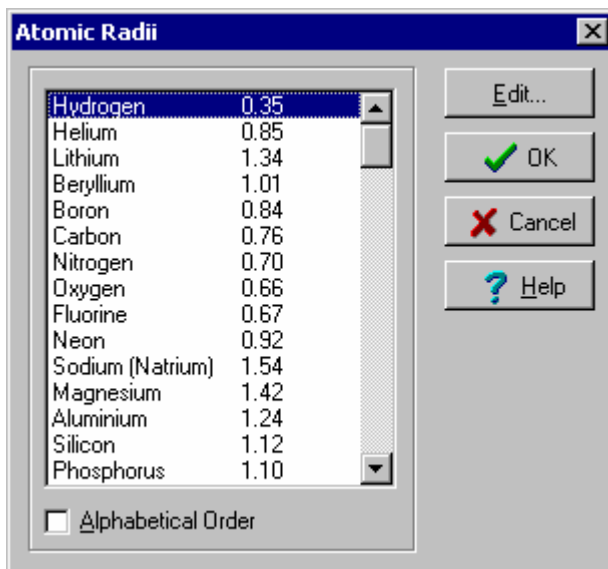
2. To view the currently set radius of any element, click it in the list. In the right column the corresponding value is highlighted.

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3. To change the atom radius for an element, double-click it in the list and type the new value, e.g., *0.5*, in the **Change Radius** box that appears:
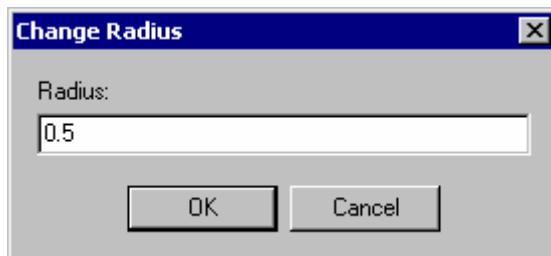

4. Click **OK** to save changes.

> **Note**   The atomic radius is expressed in relative units.

5. As soon as the changes are made in the **Atomic Radii** dialog box, click **OK**. Next time you start ACD/3D Viewer, the default values will be reset to their previous values. For more details on how to save and load default settings, refer to Section 3.4.

3.3.9 Changing the Display of Atom Radius

1. Click **Increase Atoms' Radii by 5%** . Each additional click on this button increases the radii of all displayed atoms by 5%.

2. Click **Decrease Atoms' Radii by 5%** to decrease the radii of all displayed atoms by 5%.

> **Tip**   These tools do not affect the actual radii of atoms (those specified in the **Atomic Radii** dialog box), but only change the display.

3.4 Saving and Loading View Settings

You can save the settings that you have specified during the current work session as a .3DS file, load them from a previously saved file, and set them as a new default.

3.4.1 Saving View Settings

1. From the **Options** menu, choose **Save Settings** to display the following dialog box.
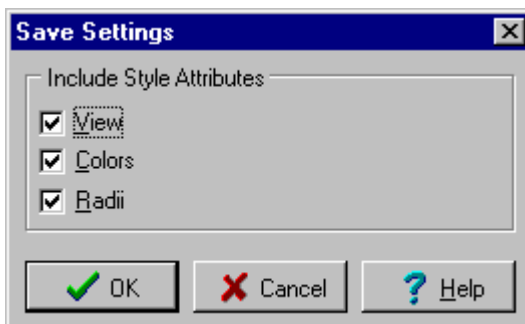
2. Select the check boxes of the attributes that you want to be saved. Note that selecting the **Radii** check box will allow you to save settings specified in the **Atomic Radii** dialog box, but not the current radius display options (see Sections 3.3.8 and 3.3.9).

3. Click **OK** and in the dialog box that appears, specify the name of the file and location (drive and directory). Note that the file should be saved with the .3DS extension.

4. Click **Save** to save the file.

3.4.2 Loading View Settings

If you have previously saved the view settings, you can load them for the current session.

1. From the **Options** menu, choose **Load Settings** to open the **Load Settings** dialog box.

2. Find the .3DS file you want to load.

3. Click **Open**. The settings contained in this file will be loaded for the current working session.

3.4.3 Setting Default View Settings

If you want to use specific settings each time you work with ACD/3D Viewer, you should set them as default ones.

1. Specify the required view settings (refer to Section 3.4).

2. To save them to a file, from the **Options** menu, choose **Save Settings**.

3. From the **Options** menu, choose **Set Default Settings** to open the **Set Default Settings** dialog box.

4. Find the file with the setting you want to set as the default.

5. Click **Open**. From this point on, each time you open ACD/3D Viewer these settings will be loaded until you specify other ones.

> **Tip** To return to the system default settings, from the **Options** menu, choose **Restore Default Settings**.

3.5 Calculating and Modifying Structural Parameters

There is a single command in ACD/3D Viewer for calculating and changing the following geometric parameters:

- Distance between two atoms,
- Bond angle, and
- Torsion angle.

While this command is selected, you can choose separate atoms. Click an atom to select it, click another atom (it may belong to another molecule) to calculate the distance between the two, click again to calculate the bond angle, and still again to calculate the torsion angle. To get a more thorough grasp of this option, let us practice calculating all of these parameters.

3.5.1 Calculating and Changing Internuclear Distances

1. Switch to the **Balls and Sticks** view mode () for a better view of the atoms.

2. From the **Tools** menu, choose **Change Geometric Parameter** or, on the Top toolbar, click **Bond Length** .
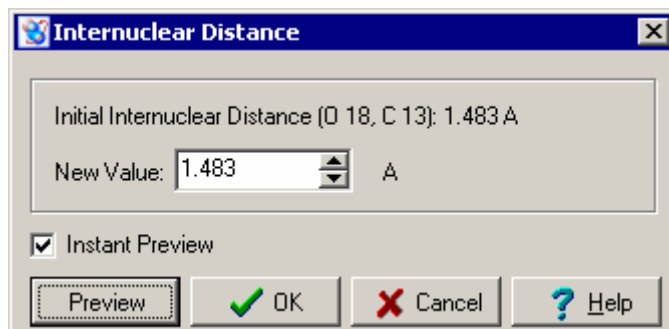
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3. Move the mouse pointer to O#18:
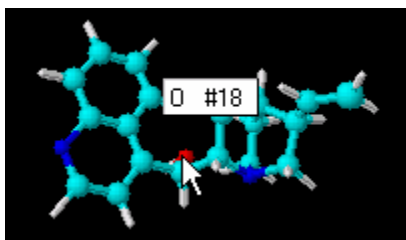
4. Click to select the atom. Note that it is highlighted with the set selection color (lime by default).
5. Move the mouse pointer to C#13:
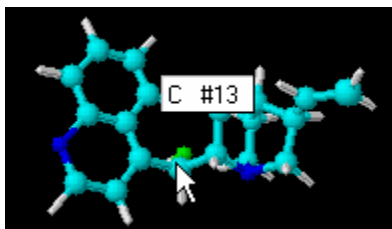
6. Click to select the second atom and the bond between the two. The **Internuclear Distance** dialog box appears:
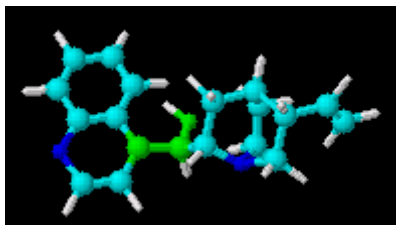

> **Tip** To change the distance, in the **New Value** box, type the desired value. If the **Instant Preview** check box is selected, the changes are immediately displayed. If the check box is not selected, after each change you need to click **Preview**. The initial distance is always present in the dialog box, so if you decide not to change the distance, you can easily return to the initial settings.
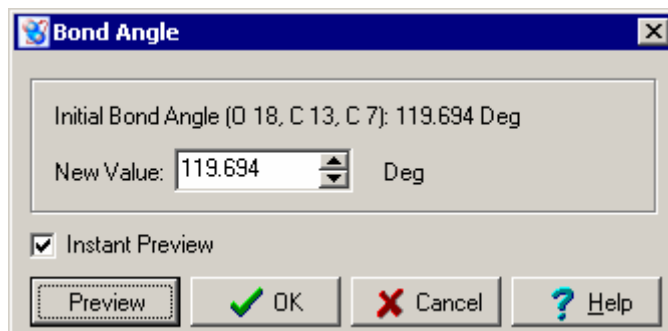
Avoid clicking **OK** in the **Internuclear Distance** dialog box; or the selection will be canceled.

3.5.2 Calculating and Changing Angles Between Two Bonds

1. From the **Tools** menu, choose **Change Geometric Parameter** or, on the Top toolbar, click
    Angle .

2. Choose the following atoms in this sequence: O#18, C#13 and C#7. By clicking the third
    atom, you define the bond angle. Below it is highlighted with lime colour:
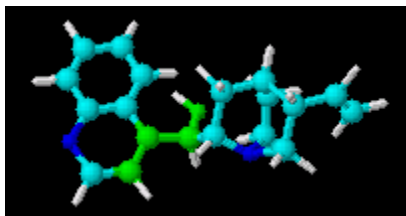

3. The **Bond Angle** dialog box appears:

> **Tip** To change the angle, in the **Bond Angle** dialog box, type the desired value in the
> **New Value** box. If the **Instant Preview** check box is selected, the changes are
> immediately applied. The initial angle is always present in the dialog box, so if you
> decide not to change the angle, you can easily return to the initial settings.
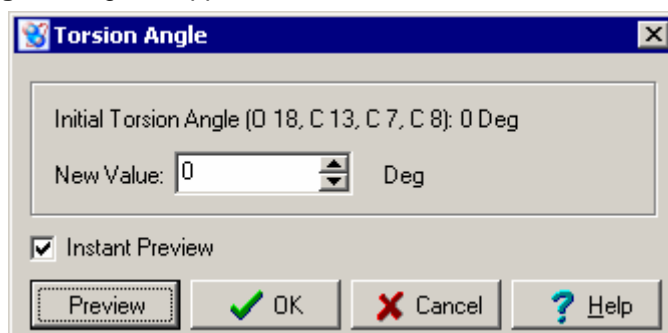
Avoid clicking **OK** in the **Bond Angle** dialog box; or the selection will be canceled.

### 3.5.3 Calculating and Changing Torsion Angles

1. From the **Tools** menu, choose **Change Geometric Parameter** or, on the Top toolbar, click **Torsion Angle** .

2. Choose the following atoms in this sequence: O#18, C#13, C#7 and C#8.

   The **Torsion Angle** dialog box appears:

3. Let us change the conformation along the C(13)-C(7) bond. In the **New Value** box, type *23*, or, if your initial value does not coincide with the above, type another value that makes the torsion angle swing around by 180 degrees. If the **Instant Preview** check box is selected, the changes are immediately applied—the bicyclic fragment is inverted with respect to the quinoline fragments:
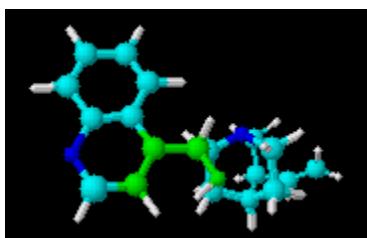
   The initial torsion angle is always present in the dialog box, so if you decide not to change the angle, you can easily return to the initial settings.

4. Click **OK** to apply the changes and close the dialog box.

5. On the Top toolbar, click **3D Optimization** to reoptimize the structure.

   | **Tip** To stop using this tool, click the **Change Geometry** button once again.

4. Creating an Animated GIF

ACD/3D Viewer,provides a set of tools to create animated .GIF files with very little effort.

The GIF file format may not be as sophisticated as Java, Flash, ActiveX, or more chemistry-oriented formats such as RasMol and Chime, but these newer applications are not as accessible to casual Web visitors who may not have the appropriate plug-ins or a connection that is fast enough. For true accessibility, a .GIF file is still the cornerstone of Web design.

Animated GIFs are a nice touch for many Web pages, whether to emphasize something on the page (e.g., the "New" revolving spheres on the ACD/Labs download page) or to show, pictorially, something which is better sketched while explaining it to someone (e.g., electron density movement in the course of a Diels-Alder reaction).

An animated .GIF file can be created by linking, in succession, one "still" or "snapshot" GIF image or *frame* after another. Each still GIF contains *nearly* the same image as the previous GIF, but is changed just enough to give the human eye the illusion of movement when one GIF is shown after the other.

The following sections describe the procedure to create animated .GIF files in ACD/3D Viewer.

4.1 Commands, Buttons, and Functions

The group of buttons for making animated .GIF files allows you to manipulate screen shots or frames, the succession of which makes up a movie. The buttons have the following functions:

| Command	Button	Function
New Frames Set		Clears the current frames (if any), thus allowing you to create a new set. If you have already attempted to create movies, your computer remembers the shot frames and adds new ones to the existing set.
Add Frame		This command adds the current screen shot to the existing set of frames (if any).
Delete Frame		This command removes the last added frame from the existing set of frames.
Auto Add Frames		Displays the **Auto Add Frames** dialog box and automatically adds the selected number of frames shot while the molecule is rotating until the set angle turn is made.

4.2 Recording Automatic Rotation

We will start with a very simple structure—butane—that is easy to draw and process.

1. In the ChemSketch window, Structure mode, draw the structure of butane:

$$CH_3$$

$$CH_3$$
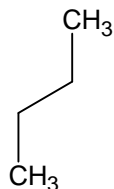
2. On the Top toolbar, click **3D Viewer** .

3. In the 3D window, click **3D Optimization** to optimize the structure.

4. Switch to the **Balls and Sticks** view ( ) and click **Increase Atom's Radii** several times to make the atoms more prominent.

5. From the **Options** menu, choose **Colors** and in the **Element** section of the dialog box, set the lime color for hydrogen and blue color for carbon. In the **Background** section, choose **White**. You should obtain something like the following:
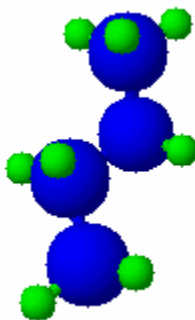
6. To start creating a new movie, on the Top toolbar, click **New Frames Set** .

7. The easiest way to record the rotation of a molecule is to record automatic rotation. On the Top toolbar, click **Auto Add Frames** .

8. In the **Auto Add Frames** dialog box, set the options as shown below:
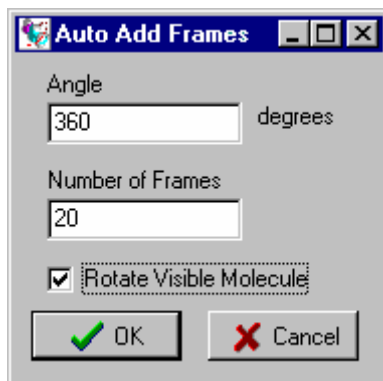
The **Angle** value defines the angle of rotation and the **Number of Frames** value regulates the number of frames that are shot for the movie.
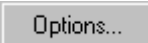
9. Click **OK** to view the rotation and close the dialog box. Later on, if you want to skip viewing the rotation, clear the **Rotate Visible Molecule** check box. 3D Viewer automatically divides the 360 degrees turn into 20 frames and records them in the appropriate succession.

> **Tip**   If you want to add a single screen shot, on the Top toolbar, click **Add Frame** ⊞ , and then move or rotate the molecule. To delete the last added frame, click **Delete Frame** ⊟ .
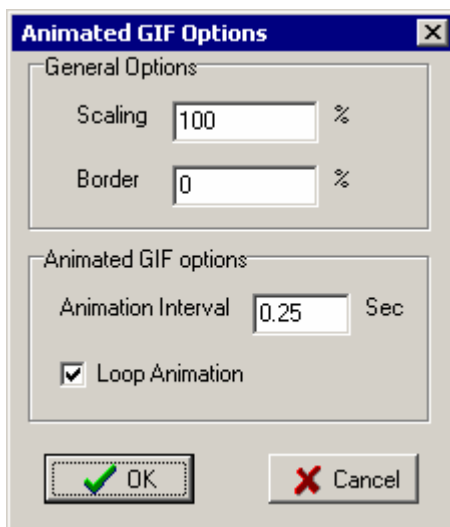
4.3 Saving Movies

The recorded frames can be easily exported to the .GIF format.

1. From the **File** menu, choose **Save As**

2. Select the file name and location.

3. In the **Save as Type** list, select *Animated .GIF Images (*.gif)*. The **Options** button `Options...` appears.

4. Click **Options** `Options...` , and in the **Animated GIF Options** dialog box, set the options as shown below:

The **Scaling** and **Border** values define the size of the structure and background area in the final .GIF file as related to those in the 3D Viewer window (in percentage). The **Animation Interval** value regulates the delay between the frames; and the **Loop Animation** check box, if selected, conditions the recurrent performance.

5. In the **Animated GIF Options** dialog box, click **OK**, and then **Save** in the **Save As** dialog box. Now, you can view the resulting .GIF file.