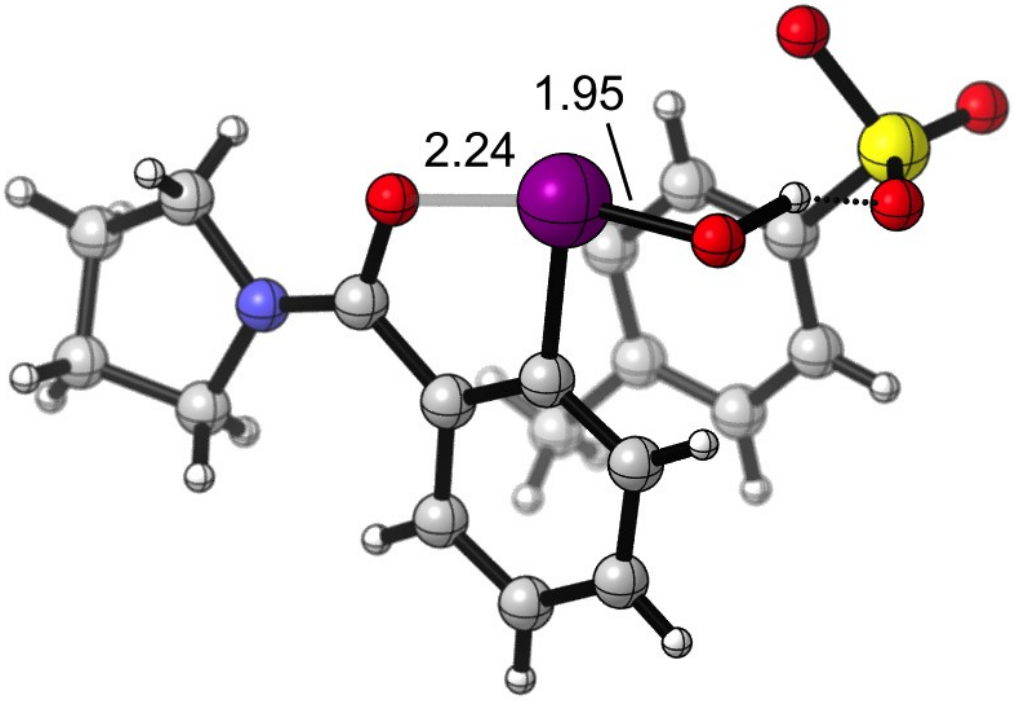
CYLview

User Manual



Rev.C

CYLview 1.0b

Disclaimer

Introduction

Thank you for trying CYLview BETA. Please email any problems or suggestions to claude_legault@cylview.org.

Installation

Windows users

Run the installer and select the installation directory.
Note: For CYLview to function properly, it must be installed with administrative privileges, as the command-line version of POVray forces the creation of the rendered image file in the CYLview directory.

Mac users

Drag and drop the CYLview.app icon in your Applications folder.

CYLview is currently only compatible with Intel based Mac computers. Moreover, the current version of CYLview runs using X11 based Tkinter. X11 server must then be installed and running properly on your computer in order to CYLview to run. The X11 server can be found on your installation CD at the following location:

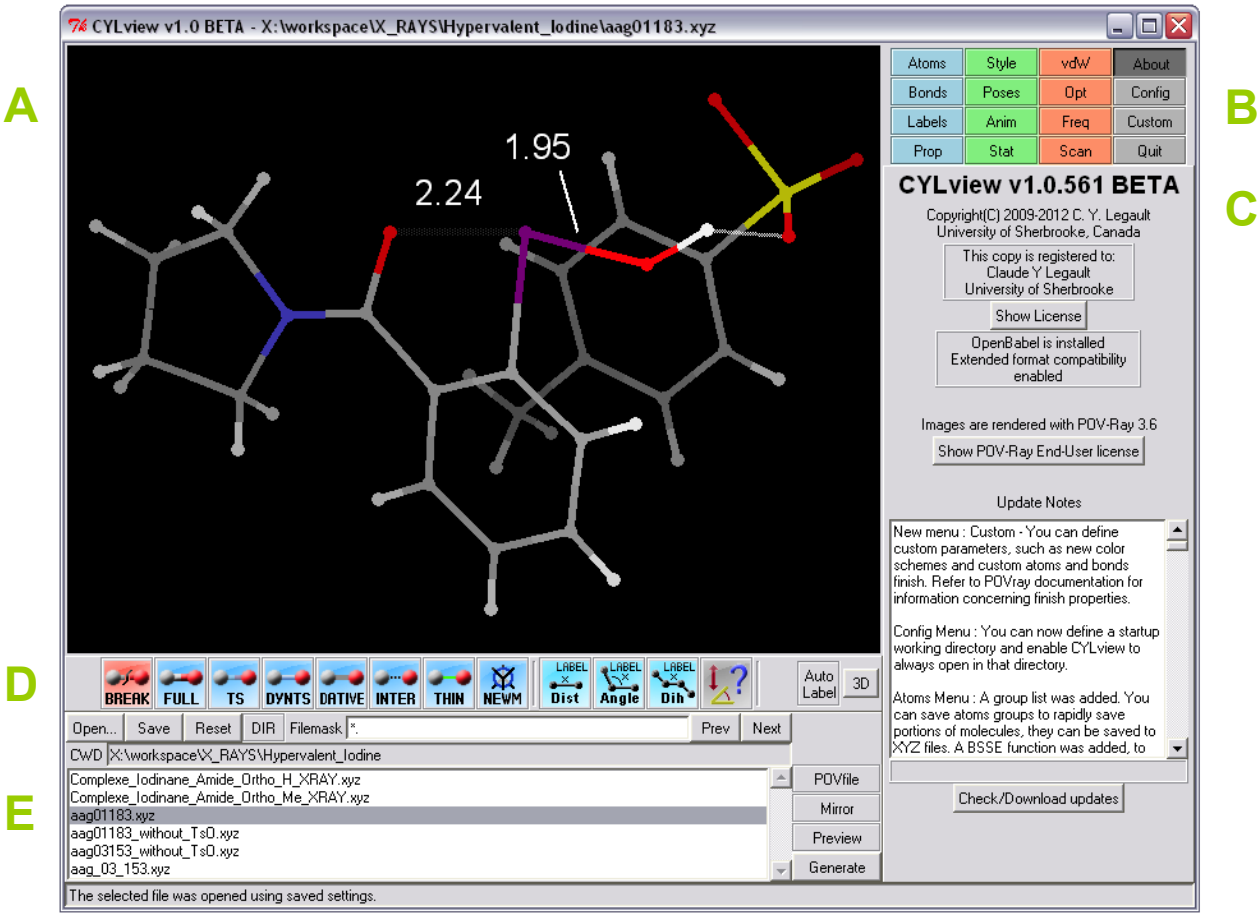
/System/Installation/Packages/X11User.pkg

Following installation, simply start the X11 server and let it run in the background.
Note: X11 server should be installed by default on Mac OS Leopard (10.5) systems. However 10.5.6+ users might have to install XQuartz (http://xquartz.macosforge.org)

OpenBabel

CYLview can use the file conversion capabilities of OpenBabel. If you have OpenBabel installed on your computer, CYLview will automatically use it to open 90 file formats. You can obtain OpenBabel at http://openbabel.org/wiki/Install.

Overview of the Interface



CYLview was designed to integrate all its features into a single window, preventing unecessary dispersion of various workspaces and toolbar windows around the screen. The interface is divided into 5 main sections:

A Molecular workspace

This is where the 3D representation of the molecular structure, including all the customizations (highlights, labels, etc.), will be represented.

B Menu Bar

Selecting a menu will reveal its various options underneath.

C Menu Options

All the available options for the selected menu bar will be displayed in this section.

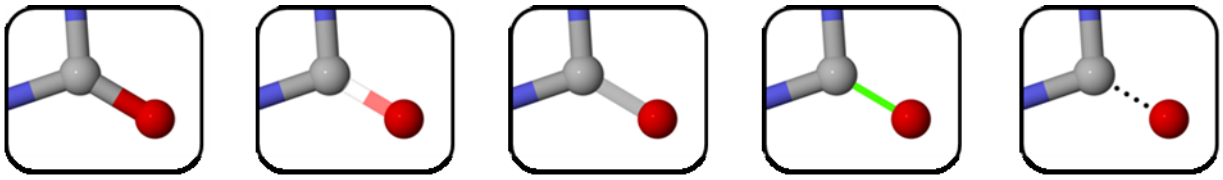
D Toolbar

They are the basic functions of CYLview. With them, it is possible to rapidly break or form bonds of different types as well as label bond distances, angles and dihedral angles. After clicking one of those buttons, the molecular workspace will enter *active selection mode* – atoms can be selected by clicking on them.

Please note that these are toggles, they will remain active until you press escape (ESC).

Bond functions: As two atoms are selected, CYLview will perform the action of the button currently selected. Here are the functions:

Break	Remove the bond between the selected atoms
Full	Create a full bond.
TS	Create a either semi-transparent or dashed bond.
DYNTS	Create a dynamic TS bond, its appearance is modified as the atom-atom distance changes. This is useful to make molecular dynamics or IRC movies.
Dative	Create a semi-transparent grey bond.
Inter	Create a black dotted interaction bond.
Thin	Create a thin bright green bond.
Newm	Create a Newman projection on the selected bond.



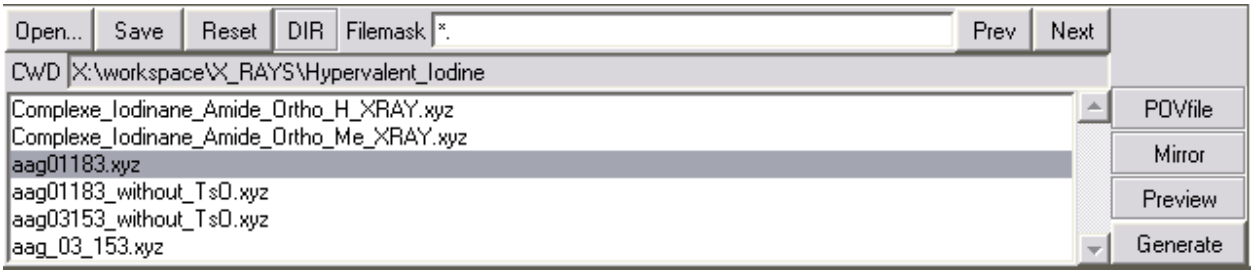
Label functions: CYLview will label bond distances, angles and dihedral angles. The label will be created once enough atoms are selected to make the measurement.

? Button: CYLview will return a measurement value, as two to four atoms are selected, which will result automatically in a value of distance, angle or dihedral angle.

Auto Label: This is a toggle that will activate auto-labeling. When enabled, it will automatically add a distance label to any bond that is created.

3D: Toggle this button to generate red-cyan anaglyphs of your structures.

E File Browser



The file browser has been designed to enable the user to rapidly move between different structures files in a subdirectory.

Open...: Open a classical Dialog window to open a single file. Following the opening, the file browser will show the content of the directory where the opened file resides.

Save: Manually save the custom settings for the structure currently loaded. *This can be done automatically (see Config Menu)*

Reset: Remove all custom settings and reload structure from the selected file.

DIR: Toggle that enable an exclusive view of the directories, in order to rapidly move between them. When the desired directory has been found, unselect the **DIR** toggle to return to the normal file listing.

Filemask: Type any filemask in the entry case to dynamically filter the files visible in the browser.

Prev and **Next**: Move to previous or next file in the file browser list.

POVfile: Generate a POVray file to render later. The extension is .CYLPOV and contains the desired resolution in the comments at the beginning of the POVray file.

Mirror: Toggle that will convert the current structure to its mirror image.

Preview: Toggle that will render the structure in the molecular workspace. The Preview will unselect itself as soon as a different menu or a toolbar function is selected or the structure is moved. No image file will be generated in the directory

Generate: This will render an image (PNG format) in the working directory. The resolution of the image will be determined by the size of the molecular workspace multiplied by the render factor (*see Config menu*). The image will not be shown in the molecular workspace when complete.

Mouse Functions

By default, the basic functions in the molecular workspace are:

Left Button: Rotate
Control-Left Button: Z-Rotate
Shift-Left Button: Rectangle Selection (only in active mode to select atoms)
Middle Button: Translate
Right Button: Zoom

In the file browser:

Left Button: Select file
Right Button: Context menu to rapidly rename the selected file with a prefix (OK_, BAD_, LOWEST_, and DUPLICATE_). This is useful to rapidly evaluate output files and remove problematic files.

*If the **One Button Mouse** is checked in the *Config menu*, the functions are:

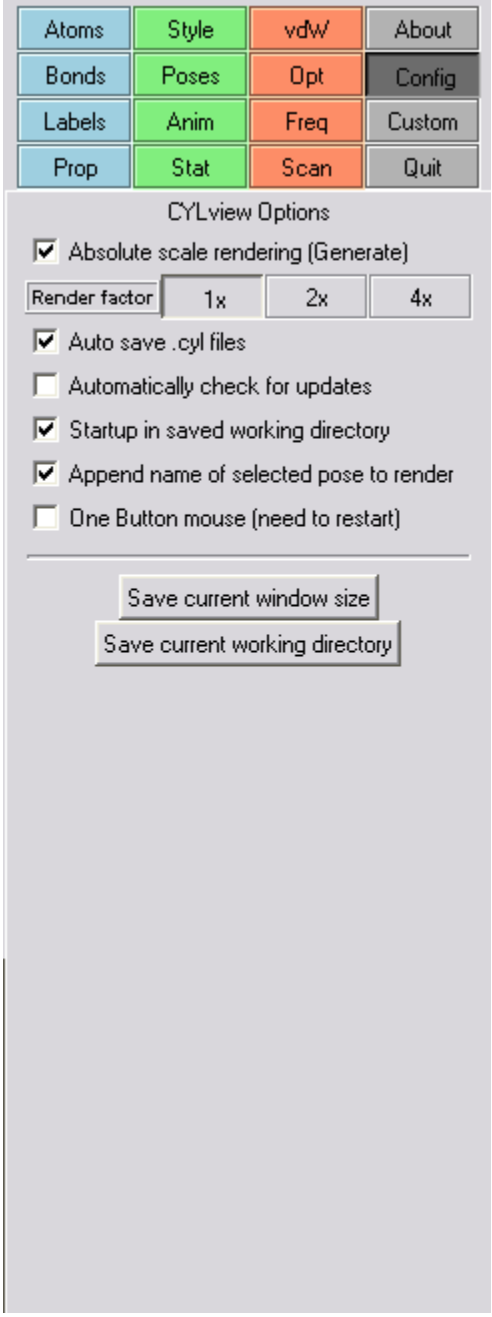
Left Button: Rotate
Shift-Left Button: Rectangle Selection (only in active mode to select atoms)
Control-Left Button: Zoom
Control-Shift-Left Button: Translate

Menus Section

About Menu

Check/Download Updates: CYLview will verify on a server and download any new components. The program then needs to be restarted in order to install the components.

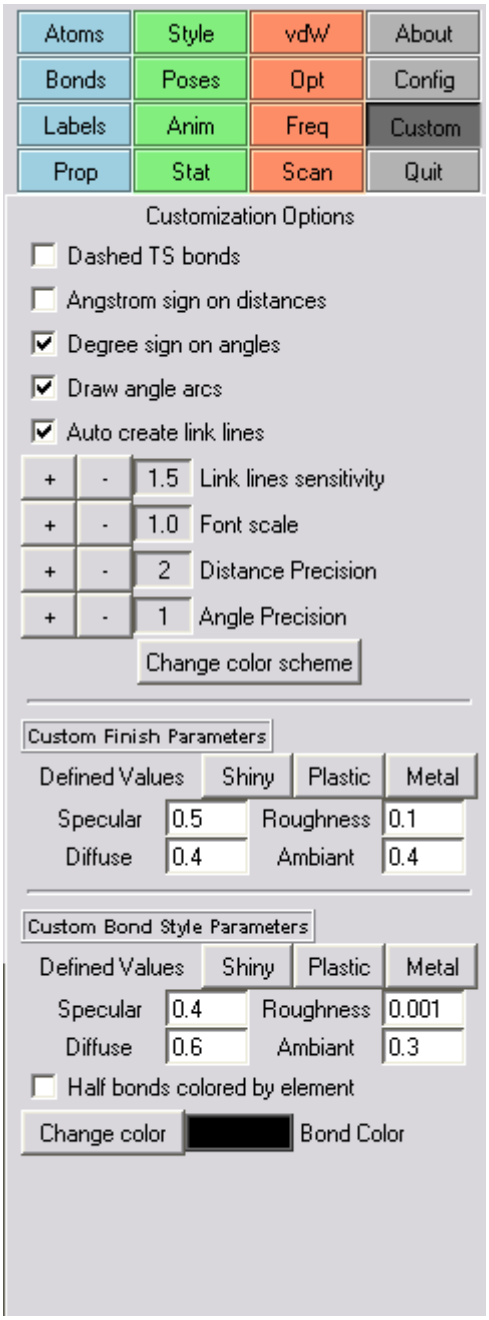
Config Menu



Absolute scale rendering: Images rendered through the Generate button will have a resolution resulting in absolute identical size structures.
Render factor: When the Generate function is used, this is a multiplication factor of the actual molecular workspace resolution applied to the rendering. Higher render factor will lead to much longer rendering time.
Auto save .cyl files: When checked, a .cyl file, containing the orientation and properties seen on screen, will be saved automatically when exiting the program or opening another structure file.
Automatically check for updates: When checked, CYLview will check for updates every time it starts. *Caution: Depending on your network connection, this may introduce a delay when you start CYLview.*
Startup in saved working directory: When checked, CYLview will use the saved working directory as the startup home directory.
Append name of selected pose to render: If a pose is selected in the Poses list (see Poses menu), its name will be added at the end of the file name when an image is rendered.
Save current window size: The current position and size of the CYLview window will be saved. CYLview will always reopen with these position and size. (Currently a problem with maximized window in Windows)
Save current working directory: The current working directory that is showed in the file browser will be saved. If the *startup in saved working directory* option is checked, this will become the initial home directory for CYLview. You can see the currently saved directory simply by moving the mouse cursor over the button, the directory will be displayed in the status bus.

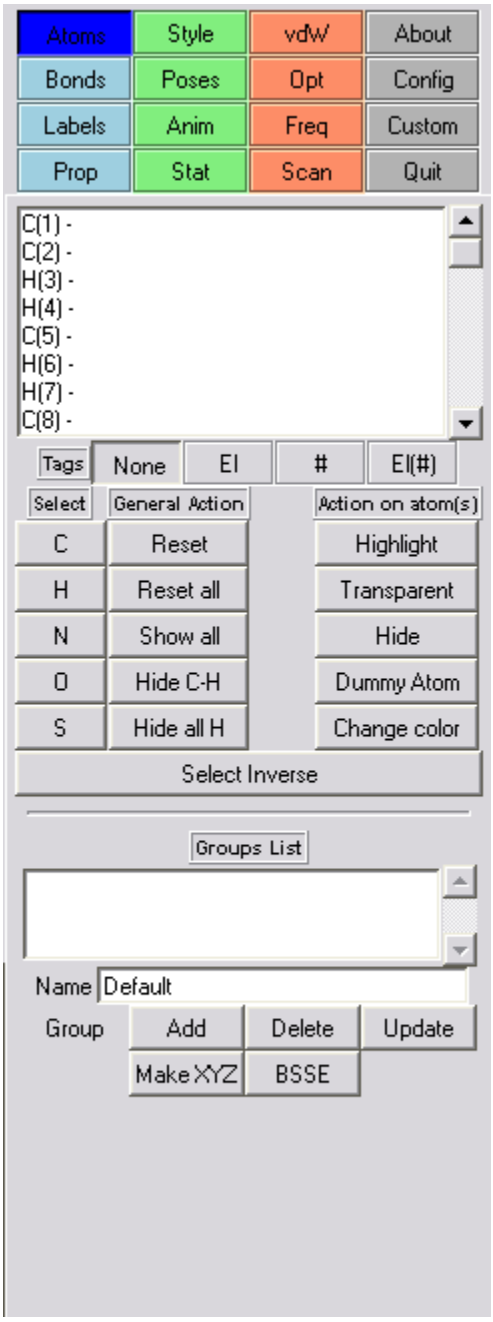
(Mac only) Generate cylview.sh: This will create a script file (cylview.sh) in your home directory that will enable you to start CYLview from a shell terminal.

Custom Menu



Dashed TS bonds: If checked, the TS bonds will appear as opaque dashed bonds. If unchecked, they will appear as semi-transparent full bonds.
Angstrom sign on distances: The angstrom symbol will be added to distance.
Degree sign on angles: The degree sign will be added to angles and dihedral angles labels.
Draw angle arcs: Angle labels will be accompanied by a thin black arc to represent their actual position.
Auto create link lines: When a label is moved over a threshold distance of its bounded atoms, CYLview will automatically add a thin black line to visually connect the label to the latters.
Link lines sensitivity: Change the distance threshold to draw the link lines.
Font scale: A general scale to modify the size of the labels on the screen
Distance precision: The number of decimal numbers on the distance labels.
Angle precision: The number of decimal numbers on the angle and dihedral angle labels.
Change color scheme: This will open a periodic table showing the default color scheme. You can change the default color by clicking on an element. This will affect the subsequently opened file.
Custom Finish Parameters: These entries can be modified to define the *Custom* finish style that can be selected in the *Style menu*. You can rapidly set starting values by using the Defined Values button. Afterward you can type in modifications. *See POVray documentation (www.povray.org) for a detailed explanation of these parameters.*
Custom Bond Style Parameters: These entries can be modified to define the finish and appearance of the *Custom* bond style that can be selected in the *Style menu*. You can rapidly set starting values by using the Defined Values button. Afterward you can type in modifications.
Half bonds colored by element: If checked, each half of a bond will be colored with respect to the connected element. Otherwise, the bond will be colored with the defined bond color.
Bond color: If the *half bonds color by element* is checked, the selected color will serve as a filter to alter the element color. Otherwise, the defined color will be used for all bonds.

Atoms Menu



Entering this menu, the molecular workspace will automatically go in active mode, meaning you can select atoms by clicking on them. Moreover, using Shift-Left Button, you can select multiple atoms using a rectangular selection mode. *Pressing escape (ESC) will remove any current selection, but will remain in active mode.*

Atoms List: Contain the list of all the atoms as well as their properties. Atoms can be selected directly through this list.

Tags: Add tags to atoms on screen

- **El** : Element
- **#** : Atom number
- **El(#)** : Element(Atom number)

Note : The tags will not show in rendering.

Select: Select the corresponding element.

Select Inverse: Invert current selection.

General Action: Action will be applied regardless of the current selection.

Reset all: Remove all special properties.

Show all: Remove hidden property.

Hide C-H: Set hidden property to C-H hydrogens.

Hide all H: Set hidden property to all hydrogens.

Action on atoms(s): Apply the selected transformation to the currently selected atoms.

Normal: Remove any special properties.

Highlight: A translucent green halo will be added to the atoms. If multiple bonded atoms are selected, the bonds will also possess the green halo.

Transparent: Selected atoms, as well as any bond connecting them, will be rendered transparent.

Hide: Selected atoms, as well as any bond connecting them, will be hidden.

Dummy Atom: Create a ghost atom that is a centroid of all the currently selected atoms. This atom will show as light yellow on screen but will be invisible in rendering. Useful for creating coordination bonds with Cp, Benzene and alkenes.

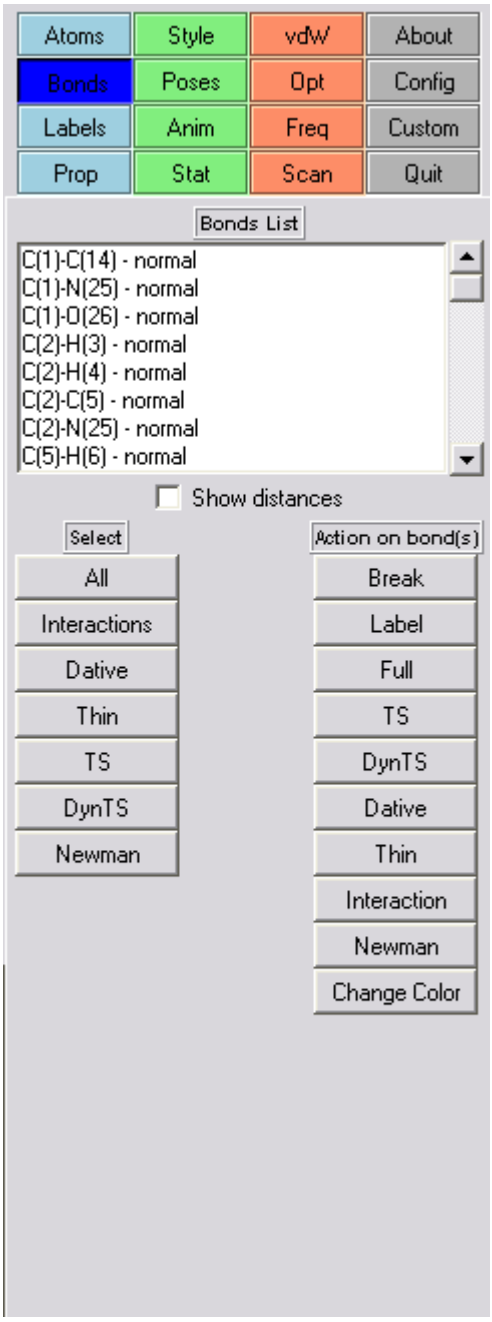
Change color: Define a custom color for the currently selected atoms.

Groups List: After selecting atoms it is possible to create an atoms group. Double clicking on a saved group will reload the selection.

Make XYZ: A XYZ file of the currently selected atoms group will be created, adding the group name as a suffix to the file. If the file already exists, it will not be overwritten.

BSSE: A formatted cartesian file with fragment information related to the existing atoms groups will be created. Useful for Counterpoise calculations in Gaussian.

Bonds Menu



In contrast to the Atoms Menu, the molecular workspace will not be in active mode in this menu. Currently, selection of the bonds can only be done in the Bonds List. *Pressing escape (ESC) will remove any current selection.*

Bonds List: Contain the list of all the bonds as well as their properties. Bonds can only be selected directly through this list.

Show distances: When checked, the bond lengths will be shown on each bond. *Note: These labels will not show when rendering.*

Select: Automatically select all bonds of the selected type.

Action on bond(s): Perform the selected action or transformation on all currently selected bonds.

Break: Remove bonds.

Label: Add distance labels.

Full: Full/normal bonds.

TS: Transition bonds.

Dative: Dative/complex bonds.

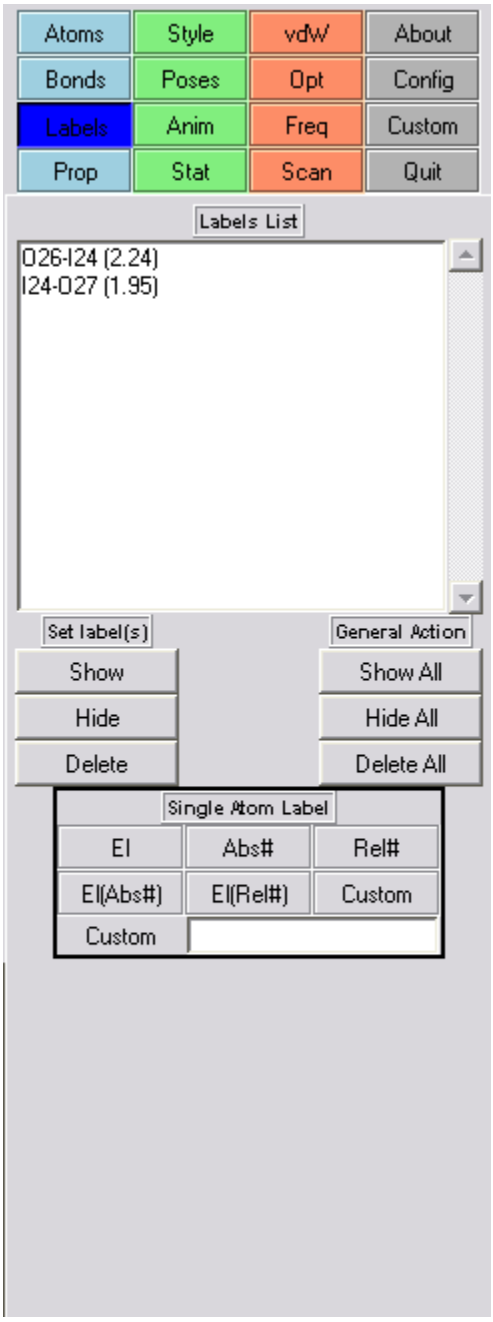
Thin: Thin green bonds.

Interaction: Black dotted bonds.

Newman: Newman projection.

Change Color: Define a custom color for the currently selected bonds.

Labels Bond



As for the Bonds menu, the labels can only be selected through the Labels List. *Pressing escape (ESC) will remove any current selection.*

Labels List: Contain the list of all the current labels. The list indicates to which atom(s) the labels are bounded, their values, and their status (e.g. hidden). *You can move the selected label(s) using the keyboard arrows. Using CTRL+arrow will move the selected label(s) using a bigger step increment.*

Set label(s): Perform the selected action on the currently selected labels.

General Action: Perform the selection action on all labels, regardless of the current selection.

Single Atom Label: When any of these toggle functions are selected, a label will be added to any atom that is selected subsequently. *Pressing (ESC) will deactivate any selected function.*

El : Element

Abs# : Absolute atom number

Rel# : Relative atom number (the value will start from 1 and increase as you select other atoms)

El(Abs#) : Element + absolute atom number in subscript

El(Rel#) : Element + relative atom number in subscript

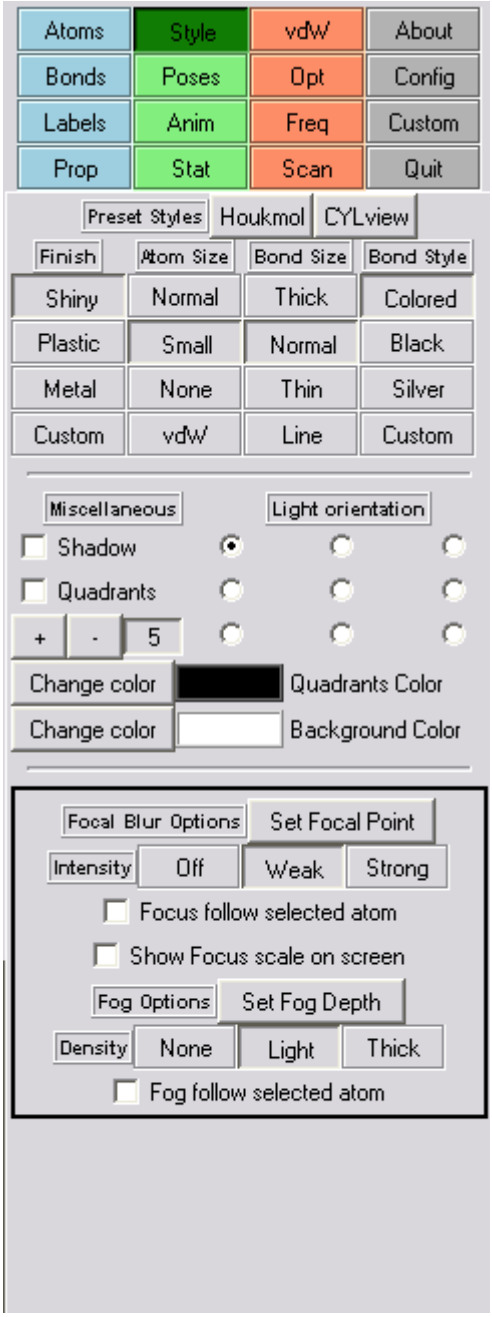
Custom : The text entered in the Custom entry below will be added as a label to the selected atom.

The custom entry currently accept basic formatting by using (__) and (**) encoding. Example:

O__7 : O_7
OC=O : $O^{C=O}$**

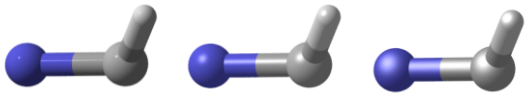
This encoding is still very primitive, you cannot return to normal text following subscript/superscript code.

Styles Menu



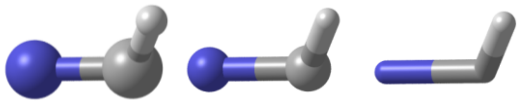
Preset styles: Automatically set up the different visual properties to reproduce the selected style. The *Custom* styles can be defined in the *Custom* menu.

Finish: Set the surface finish.



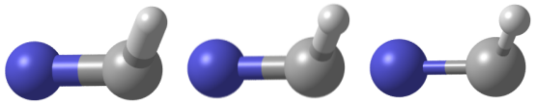
Shiny *Plastic* *Metal*

Atom Size:



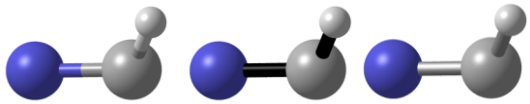
Normal *Small* *None*

Bond Size:



Thick *Normal* *Thin*

Bond Style:



Colored *Black* *Silver*

Misc (Shadow): If checked, the molecule will cast shadows.

Misc (Quadrants): If checked, quadrants will be drawn on the atoms (for Houkmol style). The thickness of the quadrants can be adjusted underneath the checkbox.

Light orientation: Position of the light with respect to the camera facing the molecule.

Quadrants Color: Define a custom quadrant color.

Background Color: Define a custom background color.

Set Focal Point (Focus): Select an atom to define the zone in focus of the rendering.

Focus Style: Set the depth of field. Strong means a more shallow depth of field resulting in stronger out of focus areas.

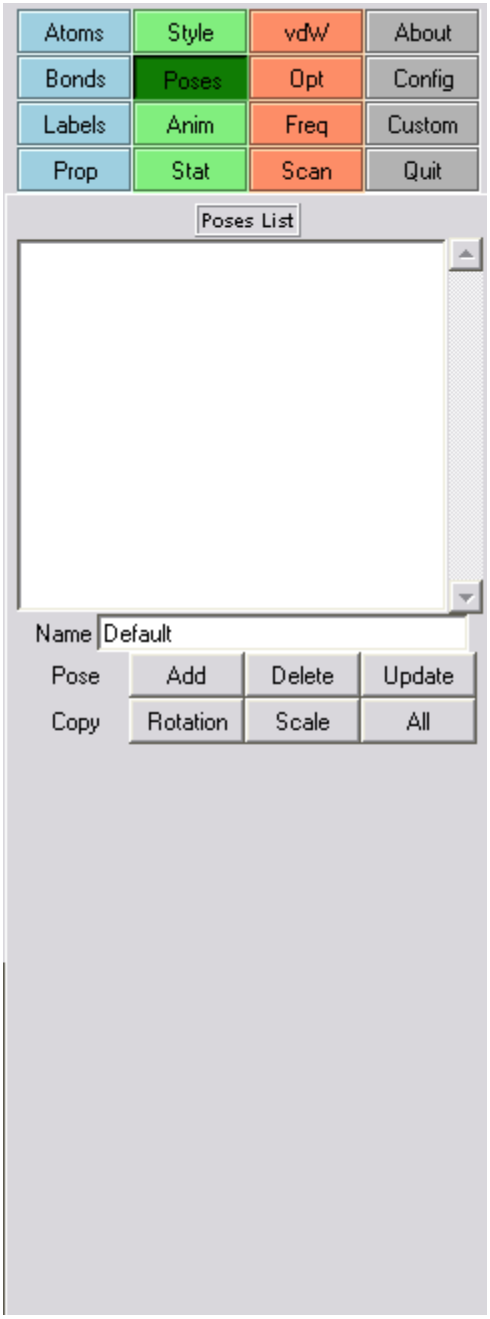
Focus follow selected atom: If checked, the position of the focal point will change according to the position of the atom selected using Set Focal Point. If unchecked, the position is fixed to the coordinates of the atom when it was selected .

Set Fog Depth: Select an atom to define the starting depth of fog in the rendering.

Fog Style: Set the density of the fog.

Fog follow selected atom: Same behavior as defined for "**Focus follow selected atom**".

Poses Menu



This menu lets you save differents orientations of your structure so that you rapidly go back to desired orientations and configurations.

Poses List: Saved poses will show in this list, with their defined names. Any pose can be reloaded by double clicking on them.

Name: When a pose is saved, it will be listed under the name set in this field.

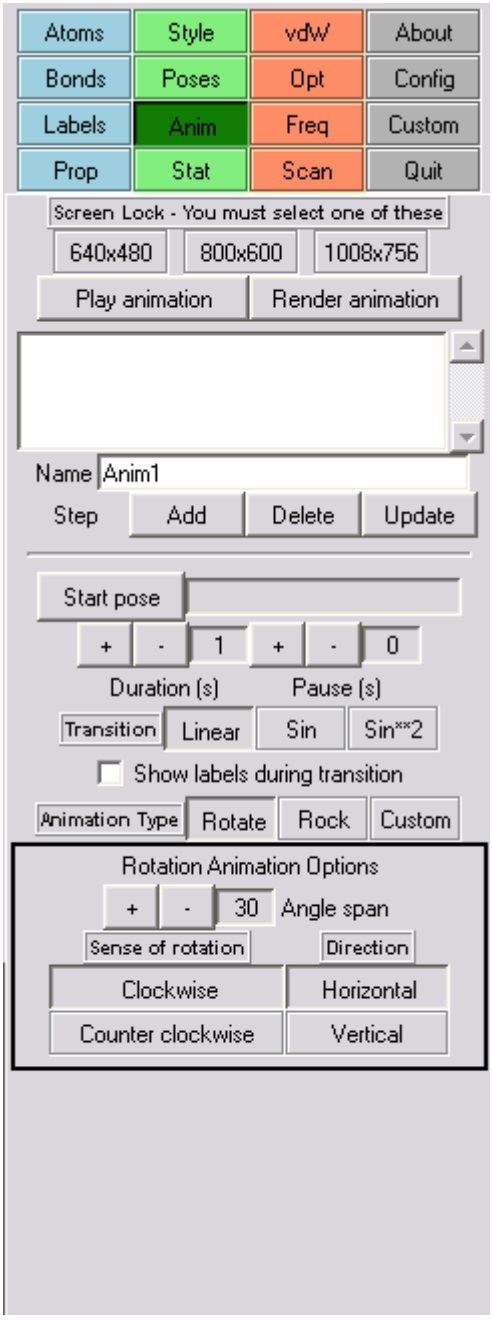
Pose: Actions to be applied on poses.

- ***Add***: Save the current orientation/settings under the name specified.
- ***Delete***: Delete the pose currently selected in the list.
- ***Update***: Update the pose currently selected with the orientation and settings of the molecule in the workspace.

Copy: Transfer specific properties of the pose currently selected in the list to the molecule in the workspace.

- ***Rotation***: Copy the rotation information to the workspace.
- ***Scale***: Copy the scale factor to the workspace.
- ***All***: Copy both properties to the workspace.

Anim Menu



This feature lets you rapidly create animation from your structure.

****** You must select one of the screen sizes before rendering the animation, as it must be a perfect 4:3 ratio. ******

Add/Delete/Update: You can build animations containing multiples steps. To add a step simply select a start pose as well as the settings desired and click **Add**. To delete a step, select it in the list and click **Delete**. To modify the properties of a step, double-click on it, change the settings, and click on **Update**.

Name: The name that will be given to the animation step in the list

Parameters common to all animation

Start Pose: Select the pose that will serve to build the animation step. It must have been created in the "Poses" Menu.

Duration: Determine the time taken for the animation.

Pause: At the end of the animation step, it will add this delay before the next step.

Transition: Determine if the movement speed is constant, sinusoidal, or squared sinusoidal. It is only applicable to rotation and custom animations.

Show labels during transition: By default, the labels are hidden during the animation. This will disable this feature.

Animation type: Selecting one of the three animation options will show extended options for the particular type:

Rotate: This will do a 360° rotation in the chosen sense around the selected axis.

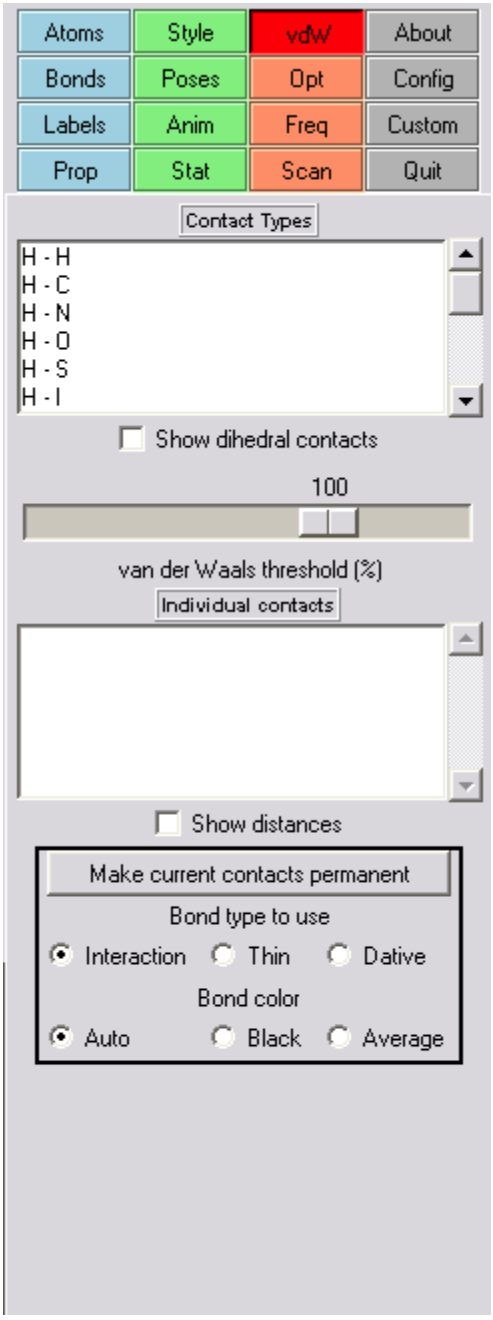
Rock: This will rock the molecule within the given angle span, around the selected axis.

Custom: This option let you generate transitions between selected poses (saved initially in the *Poses* Menu).

End Pose: Select the pose that will serve as the final orientation. CYLview will interpolate the transition path between start and and end poses.

Path: Determine if the shortest or longest route is used between the two orientations.

vdW Menu



This menu enables rapid analysis of the Steric contacts present in a structure.

Contact Types: This list is generated automatically as a structure is opened. It represents all the atom pairs in which steric contacts exist. By selecting any of these atom pairs, the contacts will show on your structure. Multiple atom pairs can be selected at the same time. To facilitate the analysis, the contacts are colored by an average of the two atom colors of the contact.

Show dihedral contacts: CYLview does not show vicinal steric contacts. By default, it does not show contacts between atoms of dihedral relationship. When checked, it will show these contacts.

van der Waals threshold: This is the threshold at which CYLview will show the contacts on screen. At 100%, the threshold is summation of the van der Waals radius of the respective atom pairs. As the threshold is lowered, only stronger contacts will show. In contrast, by using a threshold over 100%, it is possible to see probable electrostatic contacts.

Individual contacts: This list represents the contacts currently displayed on the molecule. It will show the atoms forming the contact as well as the strength of it. It is currently not possible to select specific contacts in this list.

Show distances: When checked, the contact lengths will be shown on each contact on the molecular workspace.

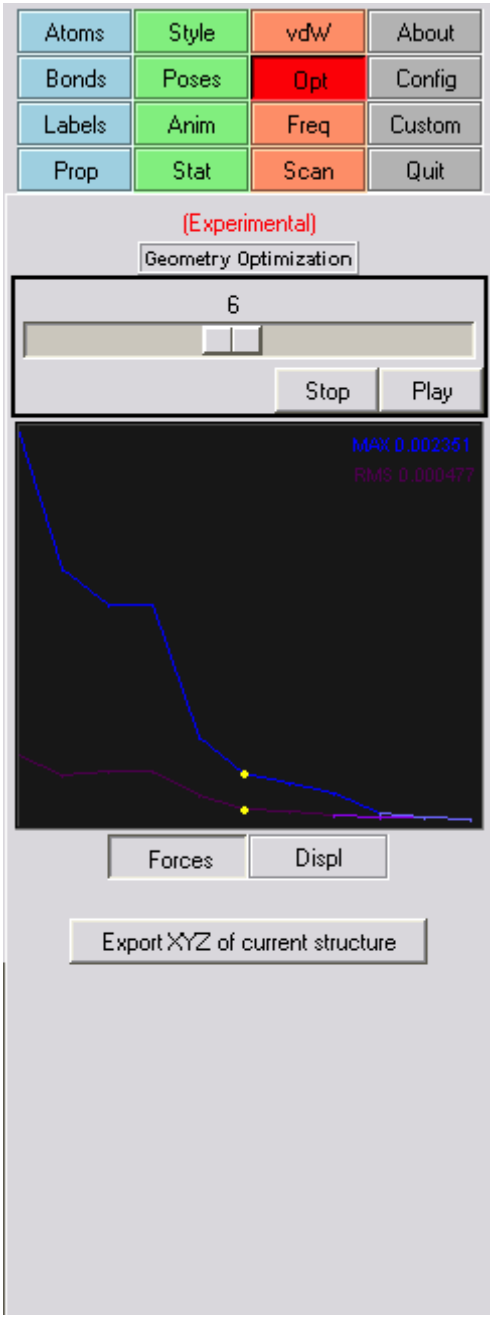
Note: The contacts bonds and their distance labels will not show when rendering.

Make current contacts permanent: This function will create bonds for all the contacts found in the Individual contacts list, so that they will be rendered.

Bond type to use: The bond type used to create the contacts.

Bond color: Auto will use black, green and grey for the interaction, thin and dative bonds, respectively. Black will force any bond type to be black and average will create the selected bond type in a color that is an average of the elements color of the atom pair.

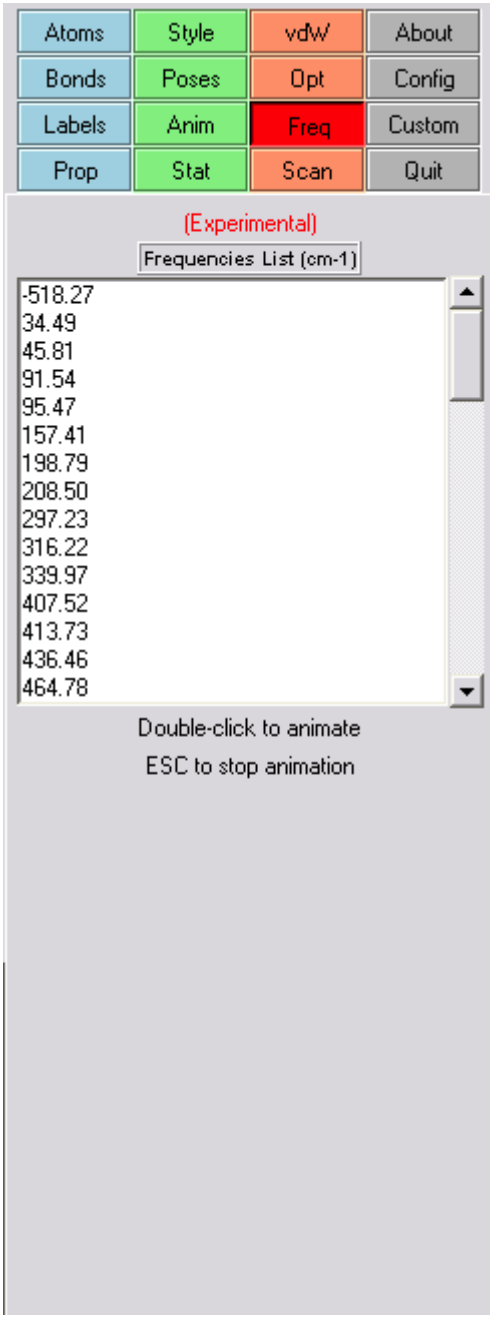
Opt Menu



With Gaussian03 and Gaussian09 output files, as you open this menu, it will check if a geometry optimization exists and display it. The slider will represent the number of optimization steps. Graph underneath will represent the Forces or Displacement.

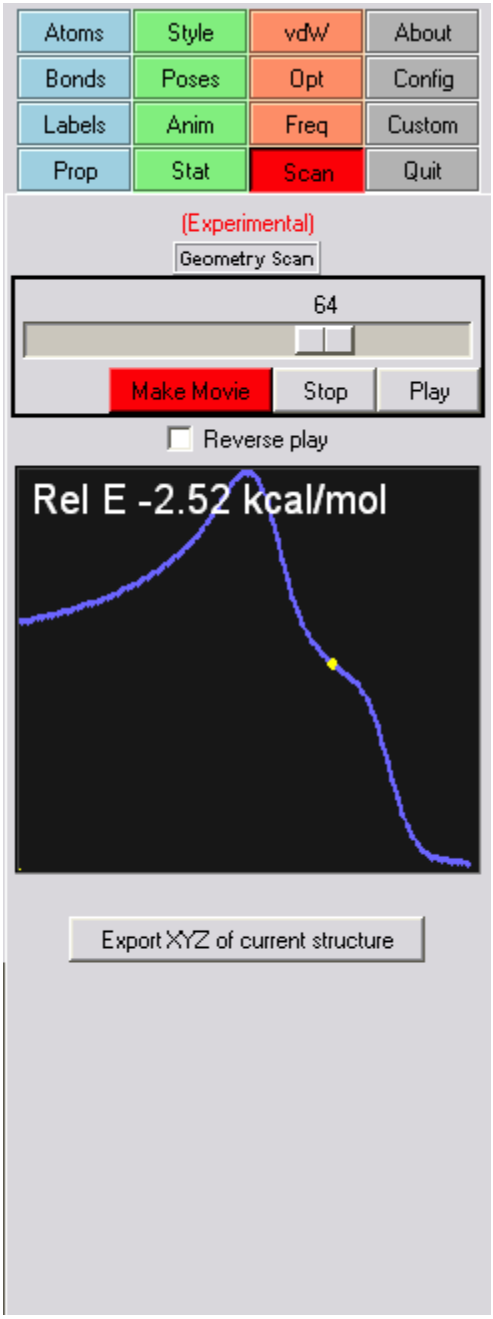
Export XYZ of current structure: The structure currently displayed (highlighted in yellow in the graph) will be saved in XYZ format. The suffix _STEP## will be added to the current file name. If the file already exists, it will not be overwritten.

Freq Menu



With Gaussian03 and Gaussian09 output files, as you open this menu, it will check if a frequency exists in the file and display the frequencies list. Double-clicking on a specific frequency mode will animate the mode on screen. Animation can be stopped by pressing escape (ESC).

Scan Menu



This module is used to open either multi-xyz files of molecular dynamics of IRC trajectories, or Gaussian03 and Gaussian09 relaxed scan files. With Gaussian output files, only converged optimization structures will be extracted and the graph will represent these points with relative energy in kcal/mol. The slider will represent the number of converged structures.

In the case of multi-xyz files, every structure must contain the exact same number of atoms. The title section of every xyz structure in a multi-xyz file is defined as:

(Number of atoms)
Title

In the title line, if an energy (in hartrees) is supplied as a second value, separated by at least a space, such as (Value1 Energy), then this energy will be used to display a relative energy value in kcal/mol.

Make Movie: A frame will be rendered for every structure displayed in the graph and a mpeg movie (30 fps) will be created.
Reverse play: The movie will be created from the last frame to the first.
Export XYZ of current structure: The structure currently displayed (highlighted in yellow in the graph) will be saved in XYZ format. The suffix _STEP## will be added to the current file name. If the file already exists, it will not be overwritten.