The QMolView user manual

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Contents

Chapter 1

Introduction

1.1 Description

QMolView is a molecule viewer application for Windows and the Linux desktop. QMolview can dislplay cml, xyz and Molden normal mode files. QMolView is free software. Consult the `LGPL v3` licence for more details.

1.2 Features

- Display `PSI4` and `hfscf` compatible `molden_normal_mode` files.
- Animate normal modes and display normal mode vectors
- Display `xyz` files.
- Display `xyz` files with multiple frames.
- Display `cml` files.
- Export all formats in `xyz` format.

The following limitations apply in the current release:

- While `xyz` files can have multiple frames, the molecule must be identical in each frame.
- Isotopes are unsupported (all formats).
- `cml` support is limited. Coordinates, element data, connectivity, and bond order data only.
- Bond orders apply to cml files only. Other formats bonds are drawn as single bonds.

1.3 About file formats

The file formats used by QMolView are standard formats well known in the area of Chemical informatics and computational chemistry. For `cml` or `Chemical Markup Language` consult the following link for more information.

The `xyz` file format is a simple human readable format in the form of a text file. An example is shown below for hydrogen peroxide contaning 2 frames. While the `xyz` specification restricts coordinates to 6 decimal places, QMolView has no such restrictions.

```
4 # Number of atoms
Frame 1 # optional title
 O     0.630721071085    -0.324607156389    -0.003488896864 # Element, x, y, z
 O    -0.630721071085     0.324607156389    -0.003488896864 # in Angstroms
 H     1.200071476450     0.300980857923    -0.424357519334
 H    -1.200071476450    -0.300980857923    -0.424357519334
4                                                          # Start of frame 2
Frame 2
 O     0.619372634413    -0.309156671276     0.046326728173
 O    -0.619372634413     0.309156671276     0.046326728173
 H     1.133733449599     0.279292450602    -0.474173144371
 H    -1.133733449599    -0.279292450602    -0.474173144371 # End of file.
```

Normal mode files with extension `molden_normal_modes` follow the format described in Molden formats. An example listing is shown below for carbon dioxide.

```
[Molden Format] # header

[FREQ] # frequencies in wavenumbers
      593.1235970630
      593.1235970630
     1397.7986066624
     2329.7215133807


[FR-COORD]
 O       0.0000000000       0.0000000000       2.1888379825 # element x, y, z
 C      -0.0000000000      -0.0000000000       0.0000000000 # in units of bohr
 O       0.0000000000       0.0000000000      -2.1888379825 # precision unrestricted


[FR-NORM-COORD]
Vibration 1 # Title for mode 1
      -0.0530150090       0.3271085119      -0.0000000000 # x, y, z
       0.1413284238      -0.8720121198       0.0000000000 # vectors
      -0.0530150090       0.3271085119       0.0000000000 # unmass weighted
Vibration 2 # etc
       0.3271085119       0.0530150090      -0.0000000000
      -0.8720121198      -0.1413284238       0.0000000000
       0.3271085119       0.0530150090       0.0000000000
Vibration 3
      -0.0000000000      -0.0000000000      -0.7071067812
       0.0000000000       0.0000000000      -0.0000000000
      -0.0000000000      -0.0000000000       0.7071067812
Vibration 4
       0.0000000000       0.0000000000       0.3313767791
      -0.0000000000      -0.0000000000      -0.8833905481
       0.0000000000       0.0000000000       0.3313767791

[INT] # optional (Napierian) IR intensities in km mol^-1
       68.3940958845
       68.3940958845
        0.0000000000
     1039.3950829646 # end of file
```

Raman intensities are currently ignored. Provided a third party package follows this format to the letter, said package can be used with QMolView.

1.4 Building the software

Consult the `README.md` for build instructions if compiling from source. An installer is available for windows only at this time. Linux binaries will have to be compiled from source.

Chapter 2

Using the application

2.1 The Main Window

The main application window comes with a standard menu and toolbar. If using the `GNOME` desktop in a Linux environment, by default, the menu bar will not be present; A hamburger menu can be found on the far right tool bar instead. A traditional menu bar can be enabled if preferred in preferences. The differences are fairly trivial, it means that some items will not be displayed on the tool bar, but appear in the hamburger menu instead.

The user manual will assume the default layout for windows and KDE from here onwards. Note also, that platforms such as KDE with a global menu enabled will display the menu bar in the top panel, not in the application itself.

Apart from visual differences and some additional preference settings only available in the Linux version, the application functions the same on all platforms, with the same feature set.

For the most part I hope that the manual will be somewhat redundant in terms of using the application. Extensive use of tooltips have ben implemented throughout, explaining each bit of functionality; Hover the mouse over any interactive `GUI` element and a tool tip will be displayed.

Figure 2.1 shows the main user interface elements when displaying `molden_normal_mode` file, and a `xyz` or `cml` file. Refer to these figures while reading the rest of the document when needed.

2.1.1 Menus and Toolbars

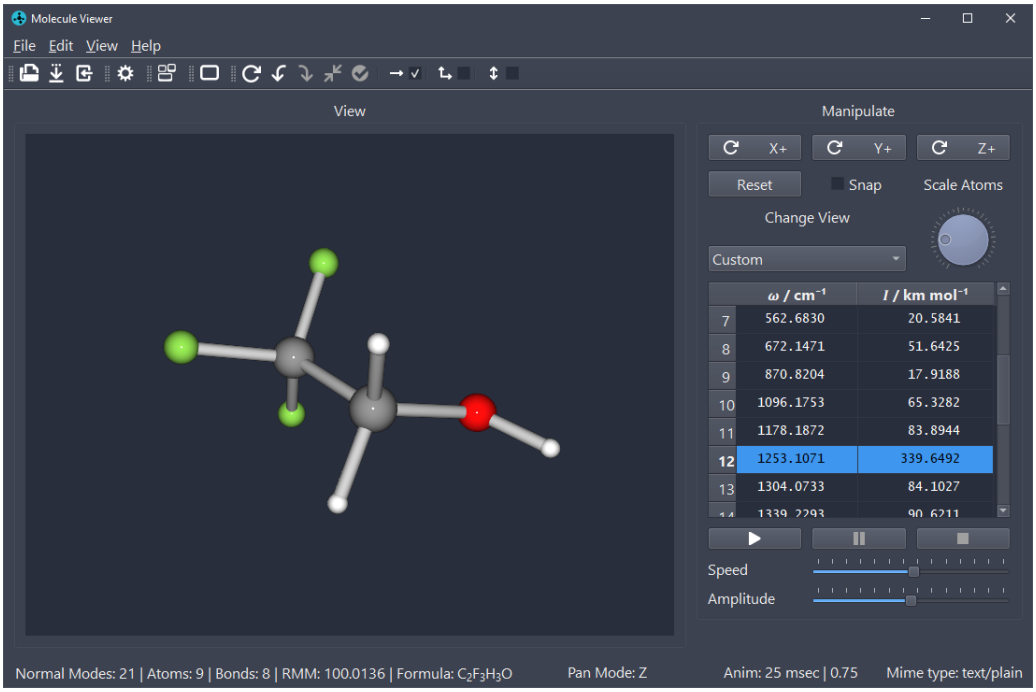
The File toolbar

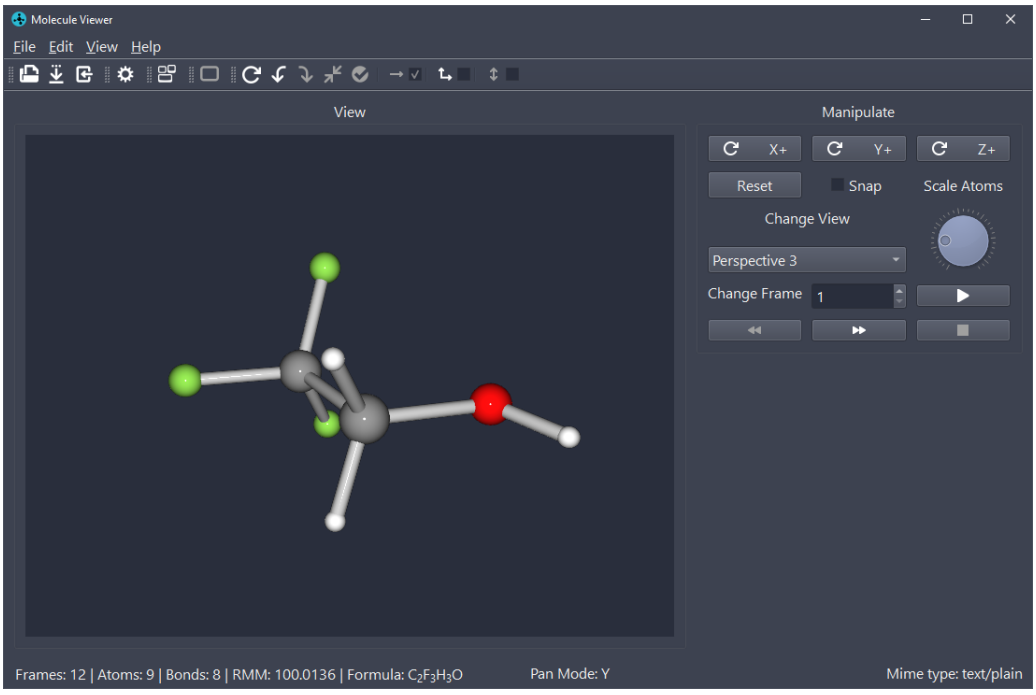
1. Pressing the `Open file` button, denoted by the icon will open the file dailog to select a molden normal mode, xyz, or cml file. This item may also be accessed via the `File` menu.

2. Pressing the `Save as` button, denoted by the icon will save the current molecule as an xyz file. For normal mode files, the current displaced geometry can also be saved. This item may also be accessed via the `File` menu.

3. Pressing the `Exit` button, denoted by the icon, will exit the application. If any custom settings were applied in "Preferences", they will be saved automatically. This item may also be accessed via the `File` menu.

Figure 2.1: The main window user interface elements when displaying a) A normal mode file b) An xyz file with multiple frames.





The Edit toolbar

Pressing the `Edit` button, denoted by the ⚙ icon will open the preferences dailog. This item may also be accessed via the `Edit` menu. See section 2.3 for more details.

The Help toolbar

Pressing the `Help` button, denoted by the icon will open the keyboard and mouse shortcuts window. Settings are fixed and cannot be changed at this time. This item may also be accessed via the `Help` menu.

The Spectrum toolbar

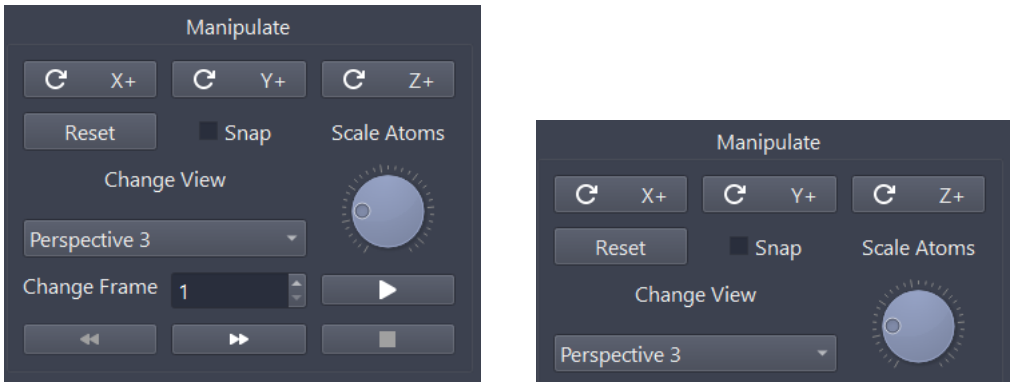
Pressing the ▢ button will open the spectrum window, provided a spectrum is available, the button will be disabled otherwise. Only applies to files with extension `molden_normal_modes`, in addition, intensity data must be present in the input file. See section 2.2 for further information on using the spectrum window. This item may also be accessed via the `View` menu.

The Control toolbar

The `Contol toolbar` is used for various functions. Some buttons may be disabled depending what functions are available at any given time, and what file type is loaded.

1. The ↻ button will toggle the rotate buttons (found in the `Manipulate` group box area) denoted by the ↻ `X+ Y+ Z+` icons from interactive to animation mode. "Interactive mode" requires the user to hold down any of the rotate buttons to rotate the molecule in the view port."Animation mode" turns all the rotate buttons into toggle buttons, so that a single press initites rotation, and another press stops the rotation animation.
2. The ↶ button will toggle the rotate buttons (found in the `Manipulate` group box area) denoted by the ↻ `X+ Y+ Z+` icons from clockwise rotation to anti-clockwise rotation. The rotate buttons will be updated to show the appropriate mode the user is currently in denoted by the ↺ `X- Y- Z-` icons.
3. The ↷ button will toggle the rotate buttons (found in the `Manipulate` group box area) denoted by the ↺ `X- Y- Z-` icons from anti-clockwise rotation to clockwise rotation. The rotate buttons will be updated to show the appropriate mode the user is currently in denoted by the ↻ `X+ Y+ Z+` icons.
4. The ↙ button becomes available when the default atom and bond scale settings have been changed by the user using the `Scale atoms` dial (found in the `Manipulate` group box area). Pressing this button will restores the default scaling.
5. The ✔ button becomes available when the default normal mode animation speed or amplitudude has been changed by the user using the `Amplitude` and/or `Speed` sliders (found in the `Manipulate` group box area). Pressing this button will restore the default animation speed and amplituide settings. Available when viewing files with extension `molden_normal_modes` only.
6. The → check box enables auto-play when selecting a normal mode from the selection view containing the normal mode listing. (found in the `Manipulate` group box area). Unchecking this box will require the user to press play each time to initiate animation when selecting a normal mode. Available when viewing files with extension `molden_normal_modes` only.

Figure 2.2: The Manipulate group box when loading a) an `xyz` file with multiple frames. b) an `xyz` or `cml` file with one frame.



7. The ↳ tri-state check box reveals the molecule fixed axes. The axes are colour coded with red corresponding to positive `X`, green positive `Y` and blue positive `Z`. Remember the mnemonic `RGB` is `XYZ`. Pressing the check box a second time makes the molecule transparent to facilitate easier viewing of the axes. Pressing the check box a third time (uncheck) hides the axes and disables transparency.

8. The ↕ tri-state check box reveals normal mode displacement vectors. The vectors are colour coded to show their relative phases, or direction of displacement. Pressing the check box a second time makes the molecule transparent to facilitate easier viewing. Pressing the check box a third time (uncheck) hides the normal mode vectors and disables transparency. Available when viewing files with extension `molden_normal_modes` only.

2.1.2 The Manipulate group box

xyz and cml files

When loading an `xyz` or `cml` file the following controls will be availabe

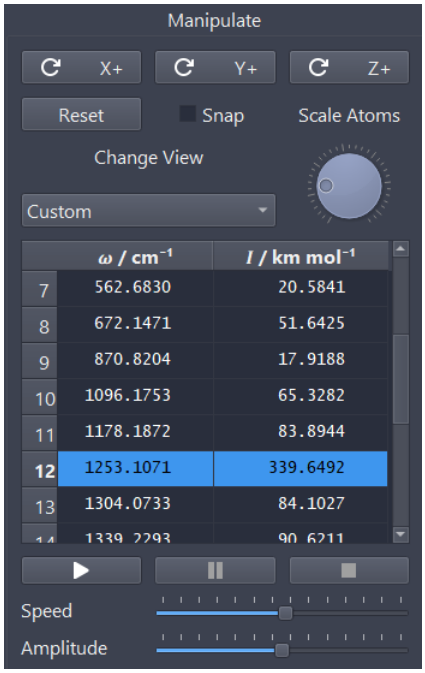
1. The rotate button denoted by the ⟳ `X+ Y+ Z+` icons allow rotation of the molecule about the `X`, `Y` and `Z` axes respectivily. The rotation centre is is the world view centre, not that of the molecule, though when the moleculde is fairly central in the view port, the difference may not be noticed. Consult item 1 how to toggle the rotate buttons from "interactive" to animation" mode.

2. The `Reset` button offers a quick way to reset the molecule to the default view, that is, the `Perspective 1` view port projection.

3. The `Snap` Check box: When enabled, snaps the molecule onto the world view origin $(0, 0, 0)$ when using the rotate buttons.

4. The `Scale atoms` dial can be used to scale the molecular model, from wire frame on the far left setting to space fill on the far right, or anything in between. The effect is purely cosmetic and has no bearing on anything else.

Figure 2.3: The Manipulate group box when loading a Molden normal mode file



5. The `Chang View` Combo box: The user can select from several view angles. There are 3 Perspective views taken from different angles, `Perspective 1`, `Perspective 2` and `Perspective 3`, as well as `Left`, `Right`, `Top`, `Bottom`, `Front`, and `Back`. All of the views can be further customised by manipulating the molecule with the mouse. See section 2.1.3 How to use the mouse inside the view port area.

The following items are only available for `xyz` file with more than one frame.
`cml` and `molden_normal_modes` files will always have one frame.

1. The `Change Frame` Spin box allows the user to select a frame number, the selection will display the molecule for the given frame number.
2. The ▶ button cycles throughall the frames, from the selected frame onwards, 'till stopped by the user.
3. The ◀◀ and ▶▶ buttons allow the user to jump to the first and last frame respectively.
4. The ■ button allows the user to stop cycling through frames. i.e. undo item 2

Normal modes files

Figure 2.3 Show the controls available when a Molden normal mode file has been loaded. In addition to the same controls available for `cml` and `xyz` files with a single frame, the following additional controls are also available in this mode:

1. A listing of normal mode frequencies and intensities, if intensities are available. When a row is selected in the table, the selected mode will begin animation, privided auto-play is enabled in the `Control` toolbar. If not, press play to begin the animation.
2. The ▶ button can be used to animate the selected mode, if it is not already in animation mode.
3. The ⏸ button can be used to pause animation of the selected mode, if it is currently running. The molecule will be frozen in whatever displaced geometry it is currently in. One can then save the displaced geometry as an `xyz` file.
4. The ■ button can be used to stop animation of the selected mode, if it is currently running. The molecule will return to its normal (non-displaced) geometry.
5. The `Speed` slider can be used to slow down or speed up a normal mode animation. The supplied animation update interval in use is printed in the status bar area (in units of milliseconds), the smaller the value, the faster the animation speed.
6. The `Amplitude` slider can be used increase the displacement of the atoms during normal mode animation. The slider is a multiplier, where 1 means the normal mode vectors are using the default scaling for displacement as supplied by the input file. Values greater than 1 increases the amplitude above normal, and vice versa. The supplied multiplier in use is displayed in the status bar area.

2.1.3 Using the View Port

The View port can be manipulated with the mouse and keyboard. The short-cuts and key bindings window gives a summary of all short-cuts and key bindings available. The short-cuts window can be accessed from the `Help` menu. The sensitivity of the keyboard and mouse responsiveness can be adjusted in the Preferences window. The Preferences window can be accessed from the `Edit` menu. Note that the view port must have the current focus for the keyboard to respond to view port inputs. Clicking on the view port once with the left mouse button will grab the focus if it currently doesn't already have the focus.

Using the mouse and keyboard

1. Hold the left mouse button and move the mouse to drag the molecule around the scene.
2. Hold the right mouse button and move the mouse to pan around the `Y` axis and tilt the molecule.
3. Hold down the `Alt` key while performing the previous action will change panning mode using the `Z` axis. The current panning mode in use is printed inside the status bar area at the bottom of the main window.
4. Holding down the left and right mouse buttons together while moving the mouse up and down will zoom into and out of the scene respectively. The same action can also be fine tuned with the mouse wheel.

Using the keyboard only

1. Use Arrow keys to move the molecule around the scene.
2. Hold down the `Alt` key while using the Arrow keys to pan around the `Y` axis and tilt the molecule.
3. Hold down the `Shift` key while using the Arrow keys to pan around the `Z` axis and tilt the molecule.
4. Press the `Escape` key to reset the scene to fit inside the view port.
5. Hold the `Page Up` key to zoom into the scene.
6. Hold the `Page Down` key to zoom out of the scene.

2.1.4 The Status Bar

The status bar is used to display several pieces of information once a file has been loaded (expressed in the form *quantity*:value|*quantity*:value...). The left section of the status bar contains the following items:

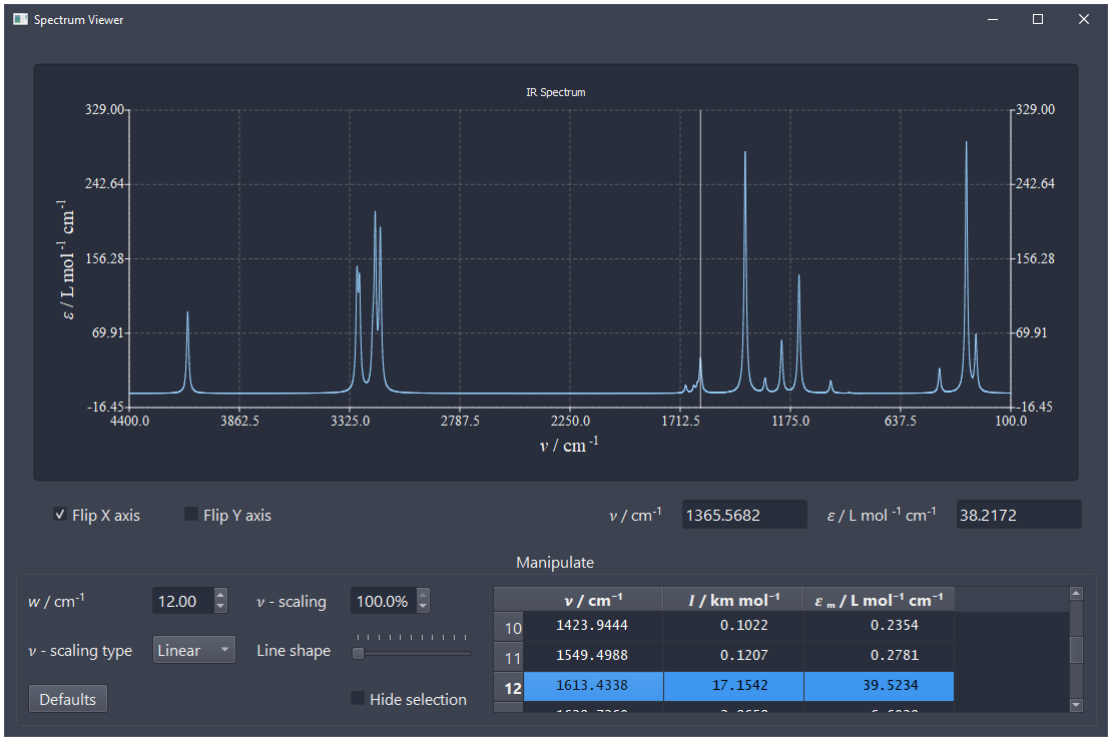
1. The number of frames in the file. In the case of `cml` and `molden_normal_modes` files this number will always be 1.
2. The number of atoms
3. The number of bonds obtained from the `cml` file, or computed by connectivity using covalent radii in the case of `xyz` and `molden_normal_modes` files.
4. The relative molecular mass.
5. The chemical formula

The middle section of the status bar contains the following items:

1. The current panning mode. By default this will display `Pan Mode:Y` meaning, when panning the scene, the `Y` axis is used. When using the mouse in the view port while holding down the `Alt` key `Pan Mode:Z` will be displayed, meaning the `Z` axis is used.
2. The animation update interval in milliseconds and the amplitude multiplier in use when animating a normal mode. This item will not be shown for `xyz` and `cml` files.

The right section of the status bar displays the MIME type. Depending what is installed on your OS this may just display as application `Mime type:text/plain` in the case of `molden_normal_modes` files, this is completely harmless, the application still knows what the file type is. `xyz` and `cml` files are typically displayed as `Mime type:chemical-x/xyz` and `Mime type:chemical-x/cml` respectively.

Figure 2.4: The Spectrum window user interface elements.



2.2 The Spectrum Window

The spectrum window becomes available when a normal mode file has been loaded and intensity data is available. All Controls are `WISYWIG`, that is to say, when any input value changes, the spectrum will be updated to reflect that change. In some cases, when a spin box input value is changed, the `Enter` key may have to be pressed to update the spectrum completely. The spectrum window offers the following controls

2.2.1 The Spectrum viewer

The spectrum viewer can be manipulated with the mouse. Use the left mouse button to drag out a rectangular area to zoom into the spectrum; This process may be repeated for increasing zoom levels. Pressing the right mouse button once resets i.e. zooms out completely.

Below the spectrum, on the left hand side, the `X` and `Y` check boxes can be used to invert the plot direction. Since IR spectra are typically displayed with decreasing wavenumber going from left to right, the X axis is flipped by default.

Below the spectrum, on the right hand side, is a motion tracker displaying the current values of the mouse cursor, representing the current values on the `X` and `Y` axis respectively.

2.2.2 The Manipulate group box

1. The w / `cm -1` spin box can be used to adjust the "The Full Width At Half Maximum" (FWHM) expressed in wavenumber units.

2. The ν `- scaling` spin box can be used to scale the `X` axis (the frequency axis). [1] A listing of scale factors for various basis sets can be obtained from here.

3. The ν `- scaling type` combo box can be used to select the scaling algorithm. The first option is to use linear scaling, the most commonly used, this means every peak in the spectrum is scaled by the same fraction. In other words, for frequency i with scale factor s, the scaled frequency is given by

$$\widetilde{\nu}_{\text{i, scaled}} = s \times \widetilde{\nu}_{\text{i}}$$

   The second less common option in my experience can prove quite useful; Using this option peaks are scaled in proportion to their wavenumber, meaning the highest peak gets the full scaling, but lower peaks get a smaller scaling. The scaling is defined such that for current frequency i, with scaling factor s, the scaled frequency is given by

$$\widetilde{\nu}_{\text{i, scaled}} = \frac{s}{1 \times \text{cm}} \times \frac{\widetilde{\nu}_{\text{i}}}{\widetilde{\nu}_{\text{max}}}$$

   where $\widetilde{\nu}_{\text{max}}$ is the highest peak.

4. The `line shape` slider allows adjustment of the peak shape in the spectrum. The default left setting assumes a pure Lorentzian line shape, the far right a pure Gaussian line shape, intermediate values assume a peak shape described by a GLS function. [2] See section 2.4 more details.

5. The `Defaults` button restores the spectrum with default settings.

6. The `Hide selection` check box can be used to hide the peak assignment line.

7. The table can be used to select and highlight a peak in the spectrum. The table will be updated accordingly when the spectrum is scaled or the FWHM value changes. Columns 2 and 3 display the IR intensities as recorded in the input file and the calculated molar absorption ϵ_{max} at maximum peak height respectively. See section 2.4 for more details.

2.3 The Preferences Window

User customisation can be applied here, such as platform specific settings, and how files are imported and exported. There are five tabs. In some cases settings will be disabled on Windows, but are only availabe in Linux, due its wide number of desktop environments.

With the exception of the `Files` Tab, all settings will be applied immediately and saved automatically. Settings are recalled for future sessions at start up. Settings can be restored to factory defaults where `Defaults` buttons are available.

[1] Since unicode does not include the $\widetilde{\nu}$ symbol to represent vibrational frequencies, it is written as ν in the application. Similarly $\widetilde{\omega}$ is written as ω.

[2] More for the show as much as anything. Don't attach too much meaning to the plotted line shape, in terms of comparing it to the true line shape of a real spectrum; Lets say, it's more of a glorified stick spectrum.

2.3.1 Appearance

The following settings are available

1. `Desktop theme` Affects the appearance and colour scheme of the application: For Linux users what appears in the combo box and what the default theme is depends on what is installed on your system. Some themes may not work as well as others. For Windows, the default theme is `Fusion Zodiac Blue`.

   Note for Linux users: When changing theme, typically the "Use standard palette" check box isn't needed, but in some cases, the Fusion theme as an example, to adopt the platform colour palette you will need to uncheck this box. If left checked the default Fusion colour scheme will be used. The same may apply to other themes.

   KDE users should always leave this box unchecked for the Plasma colour scheme to be applied. (Welcome to the chaotic world of the Linux desktop).

   You should always restart the application after a theme change.

2. `Use standard palette` See the previous item.

3. `Toolbar icon size` This setting affects the icon size on tool bars, options are small, medium, and large icons.

4. `Icon theme` It's best to leave this on the default setting. On Auto you will get white icons using a dark theme, and black icons using a light theme.

   Note for Linux users: If for whatever reason the application detected a dark theme as light incorrectly, and vice versa, you could end up with black icons on a dark theme. You'll want to override this setting to ensure the correct icon theme is applied when that happens.

2.3.2 3D View port

1. `View port brightness` Sets the light intensity in the view port.

2. `View port colour` Linux only: Sets the background colour in the view port. A custom colour can also be set.

3. `Key and mouse speed` Sets the speed of the mouse and key board when using the view port. A higher setting increases the speed with which the molecule moves when dragged, and the pan and tilt speed when rotated. The application is otherwise unaffected by this setting outside of the view port area

2.3.3 IR Spectrum

1. `Spectrum theme` You can change the spectrum colour theme and line colour using the supplied preset schemes. The default setting uses the same theme colours supplied by the `Desktop Theme` setting under the `Appearance` Tab.

2. `Spectrum line colour` When checked, the line colour will be set automatically. Unchecking this box allows the user to set a custom line colour by pressing the colour button. Note that when changing theme the check box will be reset to `Auto`.

3. `Axes title font` The font to use for labelling axes. Note that not all fonts render correctly in italics when rotated ninety degress (i.e. the `Y` axis). The default font settings work well in this regard. Axes labels follow recommended IUPAC conventions for axes labels. [3].
4. `Axes label font` The font used to print numbers beside or below axes tick marks.
5. `Show title` Whether to print "IR spectrum" as the title above the spectrum, or hide the title.

2.3.4 Platform

1. `Current Desktop` OS description. Should you wish to raise a bug report I may request what is printed in this box.
2. `Menu style` Linux only: Whether to use a traditional menu bar or a hamburger style menu. This setting will be auto detected on a per platform basis, but can be overridden here.
3. `Hide the menu bar` When using a traditional menu bar you can also hide it, since the most important actions are already accessible from the tool bar, as such, the menu bar isn't needed, unless all the tool bars are hidden. When using a hamburger menu this option will be unavailable.
4. `Use native dialogues` This setting determines whether the application wil use the dialogue windows supplied by the underlying platform, or the build-in dialogue windows, this applies to dialogues such as colour choosers, opening files, etc.

   While native dailogues fit into the underlying platform, their requested application settings are usually ignored; It is therefore recommended to use the build in dialogues where all the requested settings are guarenteed to be honoured.

2.3.5 Files

1. `Molecular connectivity` This setting determines where bonds will be drawn in the molecule. `cml` files provide this informaton as part of their input, so this setting wil be ignored.

   For `xyz` and `molden_normal_modes` connectivity is computed on the basis of covalent radii as a cut-off criterion, since the latter only has one frame this setting can also be ignored.

   This setting only comes into play for `xyz` with multiple frames. The default is the last frame, since the purpose of the application in part is to visualise geometry optimisation steps from `xyz` files, the last frame should be closest to equilibrium. If the frames go in the other direction you may want to select the first frame. In any case, there is some tolerance, where provided the structure is not too far from equilibrium, the correct connectivity will be found from either the first or last frame.
2. `Molecule fixed axes` This setting determines when the molecule is imported the axes can be sorted, This is mostly to help with alignment in the view port, where typically there is more width, than height.

   Note that when a molecule is saved as an `xyz` file, the sorted axes will also keep that order in the resultant file.

[3] The recommended convention is that variables are in italics, units are upright, and since the numbers on the axes are dimensionless, the labels should reflect that. While it is common to see something like `wavenumbers (cm` $^{-1}$`)` this is incorrect, since "wavenumbers" is not a variable, nor is it in italics, and the label implies "wavenumber `x` units", instead of "divided by", which doesn't render the axis numbers dimensionless. Essentially, axes labels follow the same rules as equations do, as for the units that appear in them, though the literature is lax on this rule.

3. `Molecule principal axes` This setting determines when the molecule is imported, whether to realign the molecule such that the principal axes coincide with the molecule fixed axes. Besides giving often a better alignment in the view port, this also affects export in the same way as the previous item.

   Should you wish to import the molecule raw, with the origanal alignment and geometry intact, you should both uncheck the `Molecule fixed axes` and `Molecule principal axes` check boxes. It should be noted that the molecule will always have the imported geometry moved to the centre of mass, and if there are multiple frames, each frame is adjusted to its centre of mass, but the principal axes are those of either the first frame, or last frame depending on what was selected in 1. In other words, strictly speaking, the principal axes are only the true principal axes of the first or last frame.

2.4 FAQ

Q: *I am using Linux: Why is the application not showing anything in the view port, or showing a transparent window, and/or becomes unresponsive.*

A: More than likely you are running Wayland session and/or using an NVIDIA GPU. You can tell if you are using Wayland by issuing the following command at the command line.

```
$env | grep land
```

If it returns Wayland you should ensure that when running the application from the command line it is started with extra argument

```
$qmolview -platform xcb
```

You may have varying degrees of success. NVIDIA wayland isn't sufficiently stable at this time, I highly recommend running an X session when using qmolview, this can usually be selected at the login screen.

Q: *I loaded an xyz file with multiple frames but I don't see any differences between frames.*

A: The differences in structures are often so small during a geometry optimisation that visually no difference may be observable in the view port. I included an example of ethane (`ethane.xyz`) where I deliberately made the `CC` bond too short, there you can clearly see the bond expanding during each step as it approaches equilibrium. If you have any doubt but want to confirm all is working check that example.

Q: *I have a normal mode running in the view port but when I want to save it the "Save as" option is not available.*

A: Pause the normal mode. The "Save as" will now be available. Moreover, the saved geometry will be the actual displaced geometry at whatever point the structure was frozen when the animation was paused. *Q*: *When I rotate or move the molecule in the view port the exported geometry appears to be the same no matter what I do.*

A: it is not a part of the software to be able to do that. The Molecule never moves or rotates when manipulating the view port with the mouse or keyboard, instead, a camera moves around the object, the actual geometry/orientation of the molecule is unaffected.

Q: *I am using KDE and have the global menu enabled, but elected to use the hamburger menu in the application, but the menu is also shown in the global menu.*

A: QMolView, while using the Qt framework on which KDE is based, does not use KDE specific features, this is how KDE handles the default Qt menu bar it appears, even though it's hidden and disabled in QMolView, call it a feature.

Q: *I am using Linux and using my favourite theme, but things look wrong.*

A: There can sometimes be a risk that third party themes can cause visual glitches in some applications, there is nothing I can do about it apart from saying, "Don't use that theme, or don't use QMolView with said theme". You can set a unique theme in `Preferences` to override the system theme, that's always an option.

Q: *Why are the maximum peak values in the spectrum sometimes different than the actual maximum peak heights in the table.*

A: The plotted spectrum can have contributions from neighbouring peaks contributing to the total or even complete overlap due to degeneracies. The value of $\epsilon_{\max}$ is calculated on the basis of an isolated peak. The spectrum may also slightly miss out on the maximum due to the step size approaching the peak width, thus missing out on the peak maximum slightly.

Q: *Where are the example files.*

A: For windows users they are in `Documents\QMolView` along with this manual, for Linux users they can be found in in `$PREFIX/share/qmolview/examples`. Compiling from source the default prefix is `/usr/local/`. For Linux flatpak installations the prefix is `/app`, and the examples are in `/app/share/qmolview/examples`, this path is only visible from within the application file dialogue since flatpaks are sand-boxed.

A note on IR intensities

A brief discussion on the methods used to plot an IR spectrum. The intensities produced by `PSI4` and `hfscf` are in units of `km mol`$^{-1}$ and in Napierian form.

$$\ln\left(\frac{I_0(\widetilde{\nu})}{I(\widetilde{\nu})}\right) = \ln(10)\log\left(\frac{I_0(\widetilde{\nu})}{I(\widetilde{\nu})}\right)$$

The Napierian form uses the natural logarithm. The definition of the Molar absorption coefficient as a function of $\widetilde{\nu}$ is given by

$$\epsilon(\widetilde{\nu}) = \frac{1}{Cd}\log\left(\frac{I_0(\widetilde{\nu})}{I(\widetilde{\nu})}\right)$$

where C is the concentration and d the path length. Using $A(\widetilde{\nu}) = \log I_0(\widetilde{\nu})/I(\widetilde{\nu})$ The integrated absorption coefficient by definition is

$$\bar{A} = \int \epsilon(\widetilde{\nu})\mathrm{d}\widetilde{\nu} = \frac{1}{Cd}\int A(\widetilde{\nu})\mathrm{d}\widetilde{\nu}$$

We assume a Lorentzian line shape of the form

$$\epsilon(\widetilde{\nu}) = \frac{2\bar{A}}{\pi}\frac{w}{(\widetilde{\nu}-\widetilde{\nu}_0)^2 - w^2}$$

Where w is the full width at half height. Converting units we obtain the result that the appropriate conversion factor is

$$\bar{A} = \frac{100}{\ln 10} \times I_{\mathrm{IR}}$$

where I_{IR} are the intensities as provided in the input file. The resultant spectrum is generated by plotting points using the function

$$\epsilon(\widetilde{\nu}) = \frac{2\times 100\times I_{\mathrm{IR}}}{\pi \ln 10}\frac{w}{(\widetilde{\nu}-\widetilde{\nu}_0)^2 - w^2}$$

When $\widetilde{\nu} = \widetilde{\nu_0}$ we obtain the peak maximum, which is what is tabulated in the spectrum window frequency table on the bottom right.

$$\epsilon_{\max} = \frac{2\times 100\times I_{\mathrm{IR}}}{w\pi \ln 10}$$

A spectral line shape can be varied by using a mixture of a Gaussian and Lorentzian line shape. It should noted that this not accurate and more for display purposes (A Voigt profile is often used to fit realistic line shapes to experimental data). In our case the form of the Gaussian Lorentzian mixture is a GLS function

$$\epsilon(\widetilde{\nu}) = AG(\widetilde{\nu}) + (1-A)L(\widetilde{\nu})$$

where A is a coefficient between 0 and 1. When $A = 0$ we have a pure Lorentzian, when $A = 1$ we have a pure Gaussian. The same value for w is used in the Gaussian and Lorentzian form. The peak height is kept constant in our implementation for convenience to see the effect when adjusting the spectrum while adding Gaussian character, so nothing else changes. Typically for peaks with larger amounts of Gaussian character such as liquids, an associated increase in w (FWHM)) would be expected to broaden the peak and lower the maximum. In general, since the true intensity is the integrated intensity, or the area under the curve, in order to keep the area constant, an increase in peak width means a decrease in peak height.