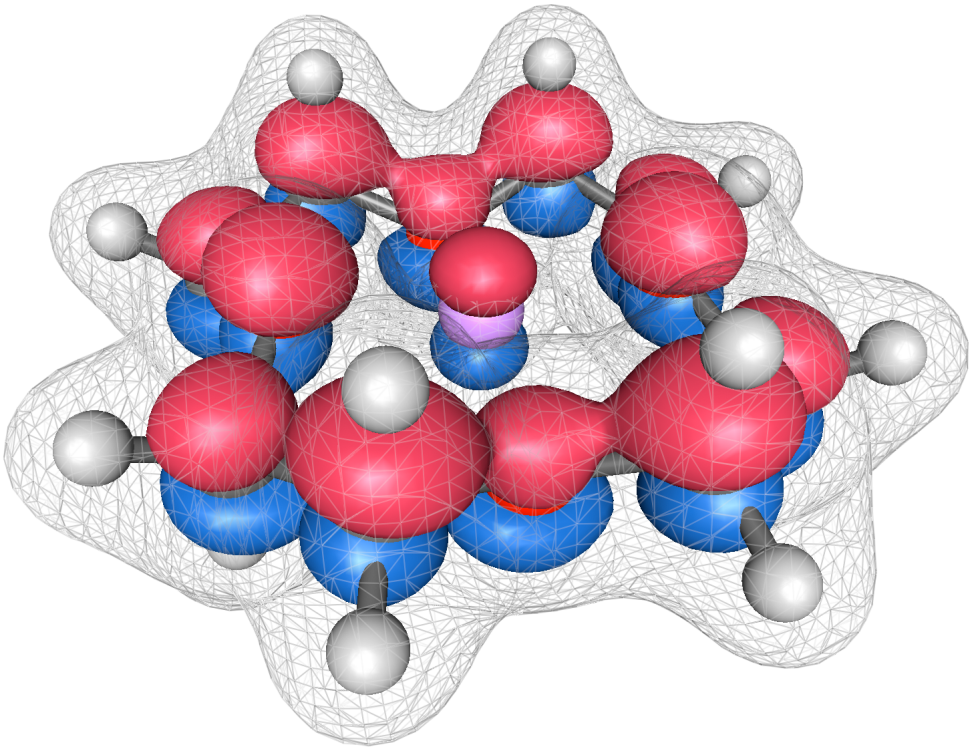
Introduction to IQmol



v2.6 (2015) Andrew Gilbert

1 Introduction

IQmol is an open-source molecular editor and visualization package that runs under Windows, Mac OS X and Linux. It can read a variety of chemical file formats including xyz, cml, pdb, mol, fchk, cube data and Q-Chem input/output. It also includes a free-form molecular builder that allows arbitrary molecular structures to be created. These structures can be optimized using molecular mechanics force fields and symmetrized to ensure the strucuture has the correct point group symmetry. A library of molecules and functional groups also exists and these can be used to facilitate building molecules.

IQmol is capable of displaying a variety of molecular properties including atomic charges, dipole moments and normal modes. Several surface types can be displayed including molecular orbitals, (spin) densities and van der Waals surfaces, and these can be colored according to an arbitrary scalar field such as the electrostatic potential. Animations are also available for vibrational frequencies and reaction and optimization pathways.

IQmol can operate as a stand-alone package, but has also been written to work seamlessly with the Q-Chem computational chemistry package. A comprehensive input file generator, the Q-Chem User Interface (QUI), provides access to most of the available options in Q-Chem, and these options are presented in an intuitive, hierarchical fashion. The generated input files can be submitted to either local or remote servers that have the Q-Chem software installed. In particular, a publicly accessable server is available that allows small (limited to approximately 5 mins) quantum chemistry calculations to be run without having to purchase and install Q-Chem.

1.1 Installation

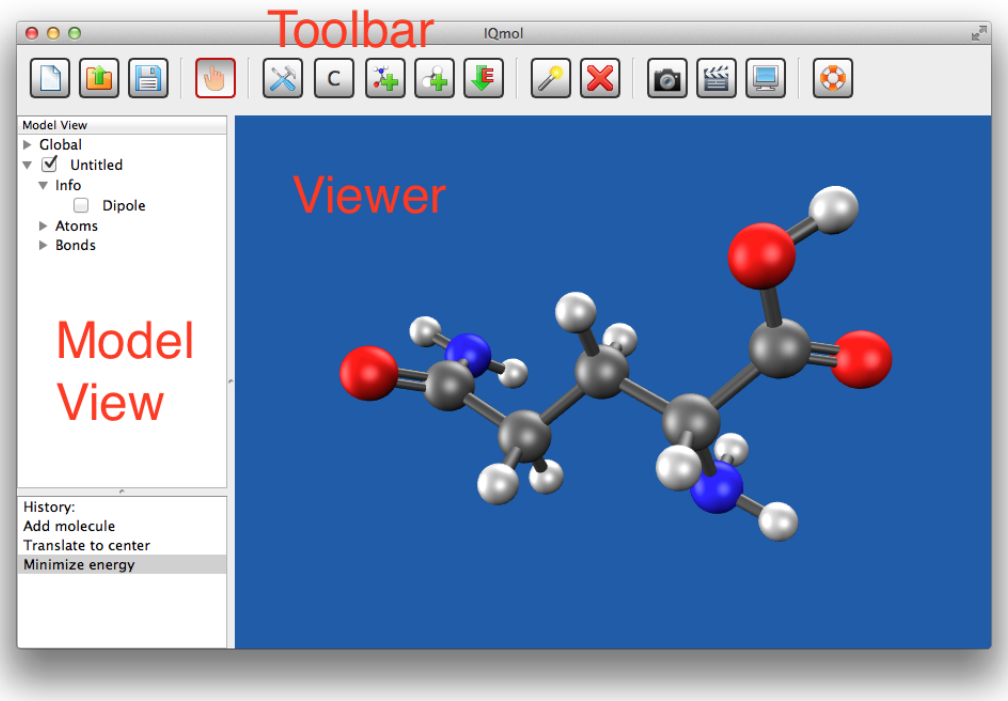
The latest version of IQmol can be downloaded from the website:

`http://iqmol.org/downloads.html`

For Mac (OS X) a disk image file is provided. Simply double click the disk image after downloading and copy the application to the Applications directory, or any other desired location.

For Windows and Linux an installer is provided that will guide you through the installation process and will also create a shortcut on your desktop.

1.2 Overview

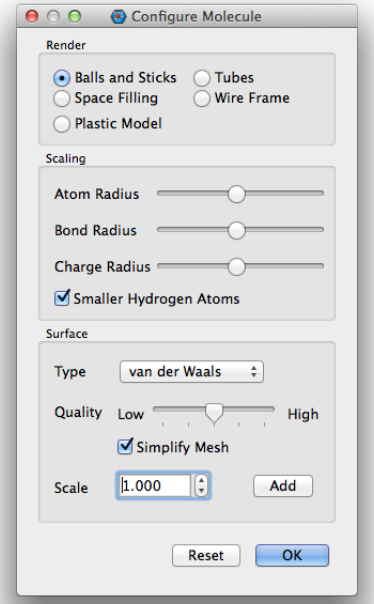


The main IQMOL window is shown above and comprises the following main parts:

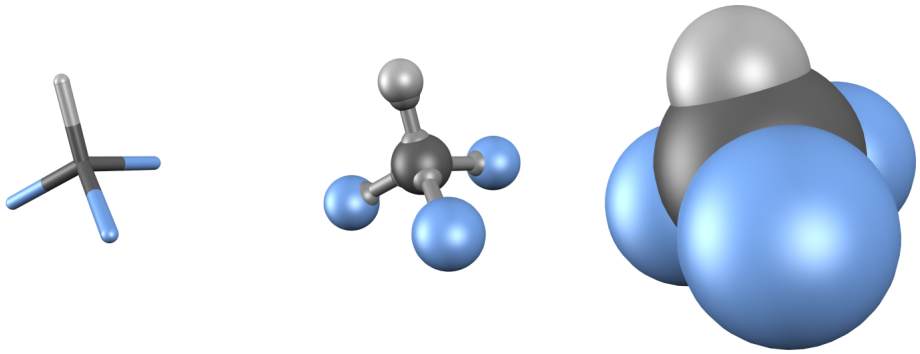
- The **Viewer** is the main part of the window and is where you can view and interact with your molecule.
- The **Toolbar** at the top provides access to common commands and allows selection between different viewer modes including manipulation, selection and building.
- The **Model View** panel provides a hierarchical view of the data that are available for the molecule.
- The **History** panel in the lower left shows a list of the most recent actions than can be undone, either by clicking on them or by using the Edit ▶ Undo menu option.

The Model View (MV) provides control over what objects are displayed in the Viewer and also allows access to configuration options for these objects. Visibility is controlled by the associated checkbox. Unchecking a checkbox causes the item and all its children to become hidden. If an item does not have a checkbox, for example a bond, then its visibility can only be controlled by items higher in the hierarchy.

The appearance of many objects can be configured by double-clicking the item in the MV. For example, double-clicking the molecule name brings up the Configure Molecule dialog:



Along with selecting different rendering options (see below), this dialog also allows several types of surface plot to be generated including van der Waals, promolecule and superposition of ionic densities (SID).



Note that several molecules can be viewed concurrently in the same Viewer and each of these can be configured separately.

2 Building Molecules

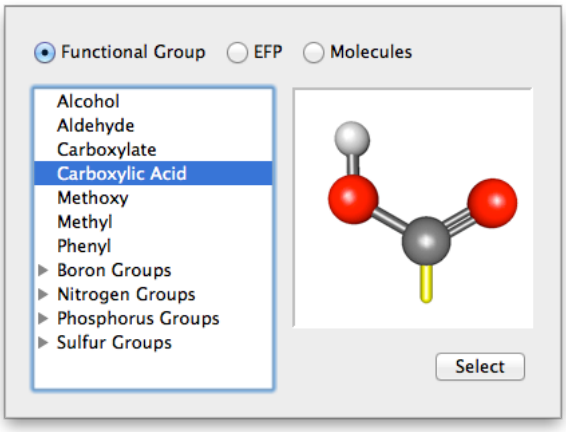
2.1 Adding Atoms and Fragments

By default, IQMOL opens in build mode. This is indicated by a red border around the  button in the Toolbar. The default build atom is indicated by the  button and can be changed by clicking on this button. A pop-up periodic table will appear from which the desired element type can be selected.

Clicking in the empty Viewer window will create an atom of the current build element. Additional atoms can be added by clicking on an existing atom and dragging the mouse. This creates a new atom bonded to the first. To create a disconnected atom, hold down the *alt* modifier key when clicking in the Viewer window. (Note that some Linux window managers use the *alt* modifier for other purposes. This behavior can be changed using System Settings ▶ Keyboard ▶ Short-cuts menu).

Bond orders can be increased by clicking and dragging between two existing atoms. If no bond exists between the two atoms, one is created. Otherwise the bond order is increased. To decrease the bond order, the bond must first be deleted and a new bond created.

Functional groups can be added by clicking the  button, ensuring the Functional Group radio button is clicked and selecting the desired group from the menu. Groups are added in the same way as atoms, *i.e.* clicking and dragging from an existing atom. The empty valence is indicated by the yellow bond and shows where the group will be connected.



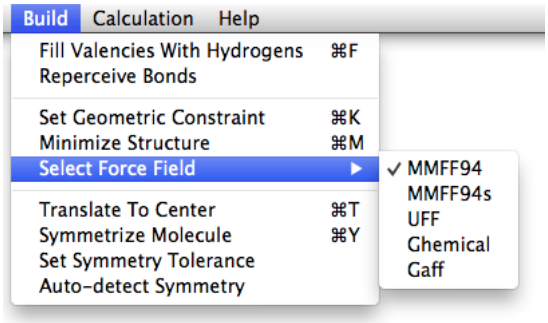
Entire molecules can be added to your system by clicking the  button, ensuring the Molecules radio button is clicked and selecting the desired molecule from the menu. Unlike the other build modes, clicking anywhere in the viewer window will add the selected molecule, (no mouse modifier is required). This allows several molecules of the same type to be added quickly, (*e.g.* for solvation), but changes the usual mouse behavior. If you

accidentally add too many molecules, use the Edit ▶ Undo menu option.

Once the backbone of the molecule has been draw the Add Hydrogens button  can be clicked to add hydrogen atoms to any unfilled valencies.

2.2 Cleaning Up Geometries

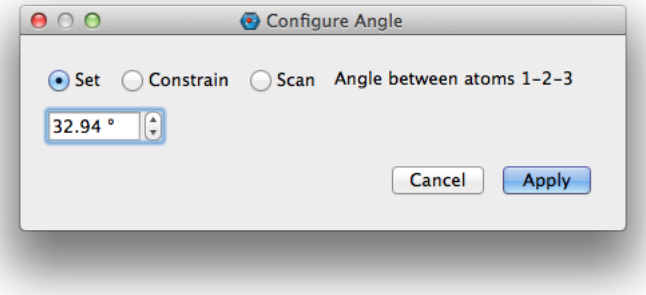
The builder in IQmol is free-form, so your initial structure may look a bit wonky. To improve the geometry, click the  button. This optimizes the geometry using a molecular mechanics (MM) force field. The default force field is the Universal Force Field (UFF) which has the advantage of being defined for most of the periodic table. However, the UFF does not perform well for systems with hydrogen bonds and in these cases it is recommended that the force field be changed by going to the Build ▶ Select Force Field menu option.



If your molecule has symmetry, the MM optimization is unlikely to find a structure with the desired symmetry. If this is the case, a nearly symmetric structure can be symmetrized using the Build ▶ Symmetrize Molecule menu option. Finding very high symmetry may require relaxing the tolerance using the Build ▶ Set Symmetry Tolerance menu option.

2.3 Specifying Geometric Parameters

Specific values for geometric parameters can be set by first selecting the atoms involved and using the Build ▶ Set Geometric Constraint menu option. A dialog will appear that allows the parameter to be either set, constrained or scanned. Constrained parameters apply to any subsequent MM optimization and are also passed through to the Q-Chem input file, if a optimization job is requested. Scan options are also passed through to Q-Chem for scan jobs.



The type of constraint depends on the number of atoms selected:

1. Fixed atom position
2. Inter-atomic distance (or select a single bond)
3. Bond angle
4. Torsion (dihedral) angle

Active constraints are visible in the Viewer and can be deactivated by clicking the adjacent checkbox in the MV.

2.4 Manipulating and selecting molecules

Select mode is activated by clicking the  button and implements the following mouse functions:

- **Left click:** Adds atom or bond to selection.
- **Click and drag:** Creates a selection rectangle, all atoms and bonds within the selection rectangle are added to the selection.
- **Right click:** Removes atom or bond from selection.

Manipulate mode is activated by clicking the  button and implements the following mouse functions:

- **Left click and drag:** Rotate the view of the molecule.
- **Middle click and drag:** Zoom in and out.
- **Right click and drag:** Translate the view of the molecule.

It is also possible to manipulate part of the molecule independently from the rest. To do this, make a selection and press and hold the *ctrl* modifier (*command* key on Mac). The mouse movements will affect only the selected atoms as follows:

- **Left click and drag:** Rotate the selected atoms about their center.
- **Right click and drag:** Translate the selected atoms.

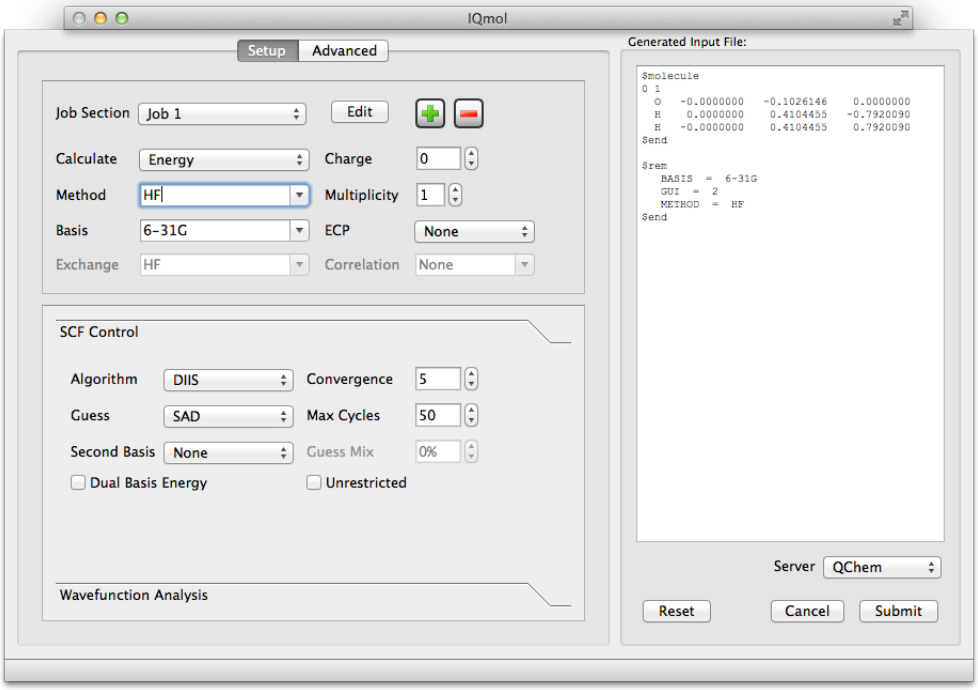
If a single bond is selected, then the mouse movements have the following effects

- **Left click and drag:** Rotate around the axis of the bond.
- **Right click and drag:** Change the length of the bond.

3 Running Q-Chem Calculations

3.1 The QUI

IQmol has a built-in input file generator for Q-Chem calculations, the QUI, that can be accessed via the Calculation ▶ Q-Chem Setup menu.

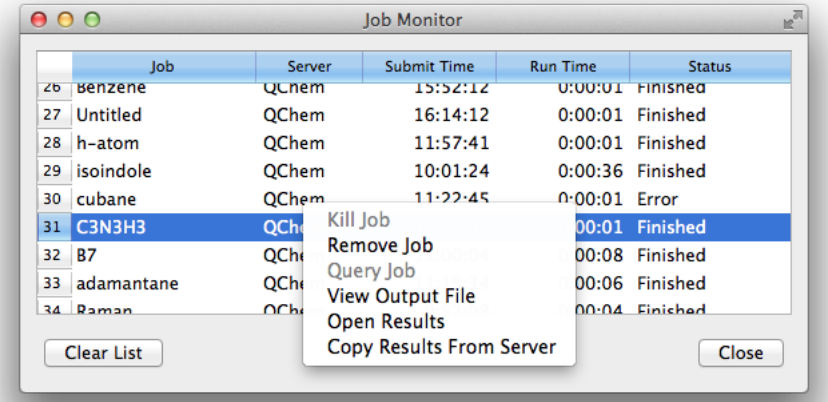


The left hand side of the QUI dialog contains controls for setting up the calculation. These are presented in a hierarchical fashion so that most commonly used options are presented in the top part of the panel, with other relevant options appearing in the lower section depending on what type of job is selected. More advanced options can be accessed via the Advanced tab. The generated input file is echoed in the panel on the right hand side of the QUI.

Clicking the Submit button will start the job running on the selected server. Once the job has completed you will be prompted to copy the results (for remote servers) before they are automatically loaded into IQmol. The ⭐ icon appears next to the molecule name in the MV when the molecule has been updated with the results of a calculation.

3.2 The Job Monitor

Submitted jobs can be monitored via the Calculation ▶ Job Monitor menu option. This brings up the Job Monitor dialog that provides information on the progress of jobs. Right-clicking a row in the Job Monitor brings up a context menu which allows running jobs to be killed or queried, and finished jobs to be opened.

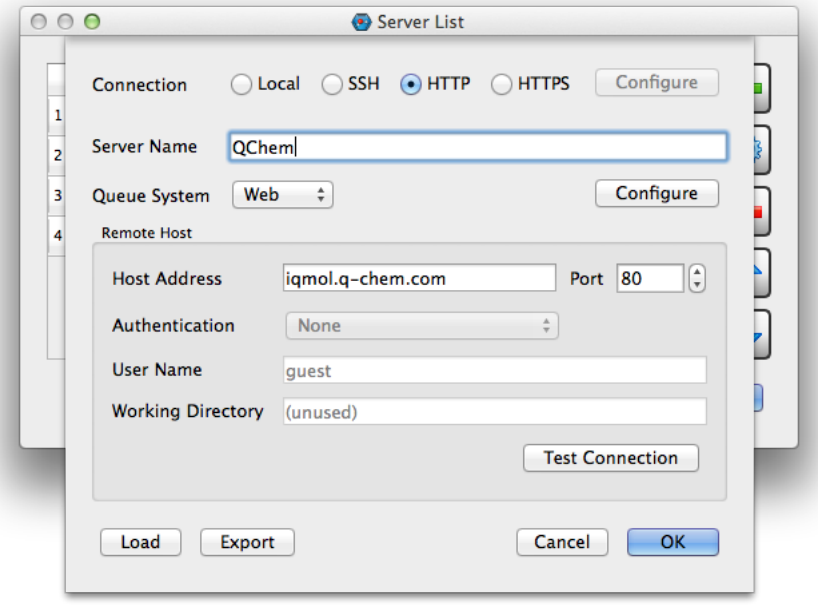


If a job has the Error status, hovering the mouse over the status will show the error message. Alternatively, double clicking the job will open the output file, if available.

3.3 Configuring Servers

By default IQmol is configured to submit jobs to the HTTP Q-Chem server in Pleasanton, California. This is a publicly available server than can be used by anyone wishing to run test calculations before purchasing the Q-Chem software. Jobs submitted to this server can access the full suite of electronic structure methods available in Q-Chem, but are time-limited to 5 minutes.

Additional servers can be configured to access other computers that have the Q-Chem software installed. These computers can be either local servers (*i.e.* the same machine as the one running IQmol) or remote servers that can be connected via SSH. To add an additional server, go to the Calculation ▶ Edit Servers menu option and click the  button.



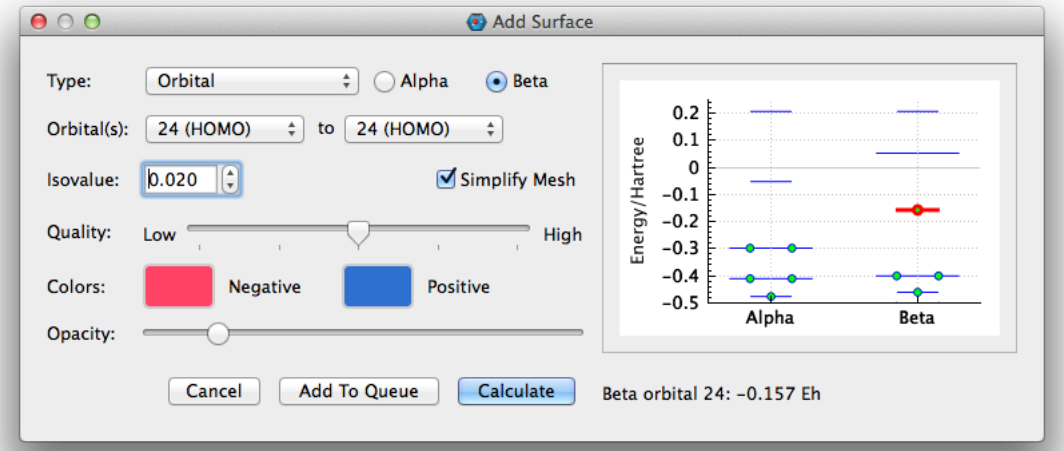
The information required to configure a server depends on its type, but default options exist for each case. The following indicates the minimum that should be considered:

- **Local:** Set the Queue System to 'Basic' unless you know you are running queuing software on the machine. Be sure the `QC` and `QCSCRATCH` variables are set to their correct values in the Run File Template, which is accessed by clicking the Configure button.
- **SSH:** The hostname and account on the target machine will be required in order to connect via SSH. Set the Authentication combo-box to 'Password Prompt' unless you have set up an alternative authentication protocol. Depending on how the target host has been set up, the Run File Template may require some editing to get it to work, but this will differ from machine to machine.
- **HTTP:** The default options should be suitable.

4 Analyzing Results

4.1 Plotting Molecular Orbitals

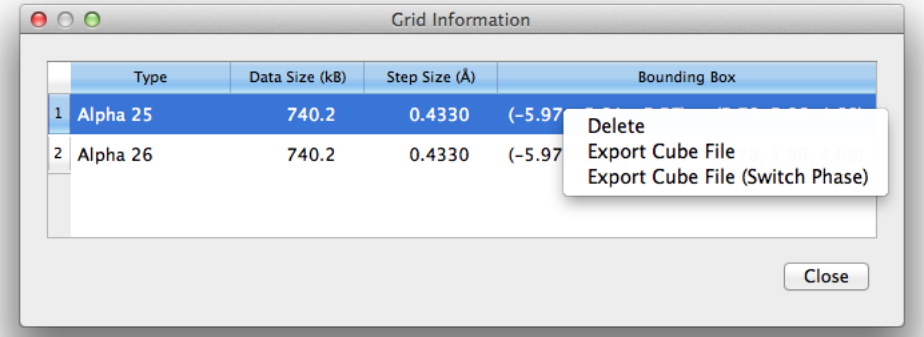
Plotting molecular orbitals (MO) requires a formatted checkpoint file (.fchk) which is generated by default when running Q-Chem calculations using IQmol (GUI rem variable should be set to 2). After opening the file, a MO Surfaces item will be available in the MV, double-clicking this brings up the Add Surface dialog:



The dialog allows both MOs and densities to be computed, and several surfaces can be computed at the same time (this is more efficient as the shell data only needs to be computed once). The quality, colors and opacity of the surfaces can be be set in the dialog, and changes to these settings are saved to the preferences as default values for future surfaces. Once computed, the individual surfaces appear as sub-items in the MV and these can be further configured by double-clicking the items in the MV.

The Add Surface dialog also contains an interactive energy level diagram. The vertical scale can be zoomed in and out using the scroll wheel (or equivalent) on the mouse. The scale can also be translated by a left click-and-drag. Individual orbitals can be selected with a left-click and this will cause the energy of the selected orbital to appear below the diagram.

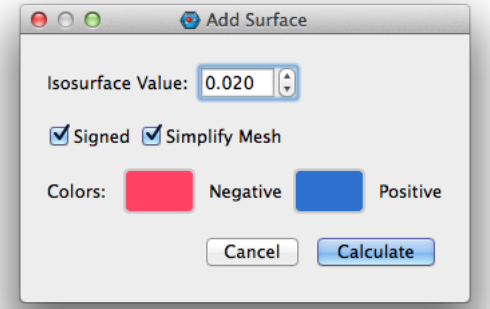
The grid data generated for each surface is stored internally so that subsequent calculations of the same surface (with different isovalues, for example) are much faster. To see what grid data is being stored, right-click on the MO Surfaces item in the MV to bring up the context menu. Selecting the Show Grid Info menu brings up the Grid Information dialog:



From this dialog it is possible to export cube files containing the grid data. Right-clicking on the desired grid brings up a context menu with the option Export Cube File option. The Switch Phase option swaps the sign of the data and may be useful when comparing two systems where the (arbitrary) phases differ. Cube files can be saved for future plotting to avoid having to recompute the data, or for reading into another plotting package.

4.2 Visualizing Cube File Data

Cube files contain volumetric data such as electron densities, molecular orbitals or electrostatic potentials (ESP). Because the data has been pre-computed, generating surfaces using them is very quick. After opening a cube file, a Cube Data item will appear in the MV, double-clicking this item brings up the Add Surface dialog:

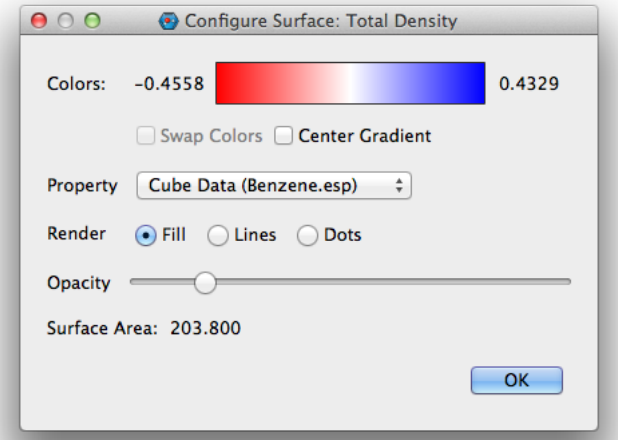


The Signed checkbox causes two isosurfaces to be generated corresponding to ± the specified isovalue, and this should be checked for data such as MOs and spin densities.

Cube file data can also be used to color a surface and this will require either two cube files (one containing the surface data and the second containing the property used to color the surface) or a cube file and a checkpoint file. In either case two files need to be loaded into the one molecule. To do this, ensure the files are in the same directory and have the same base name (everything up to the first '.'). For example, the directory might be named 'Benzene' and contain the files 'Benzene.esp.cube' and 'Benzene.fchk'. The File ▶ Open Dir menu option can be used to open the directory and both the cube and fchk files will

be loaded into the Benzene molecule in the MV.

After creating a surface, as detailed above, double-clicking the surface item will cause the Configure Surface dialog to appear:



The Property combo-box will have the cube data as one of the options, and selecting this will cause the surface to be colored according to the data in the cube file. The gradient colors can be altered by clicking inside the gradient box.

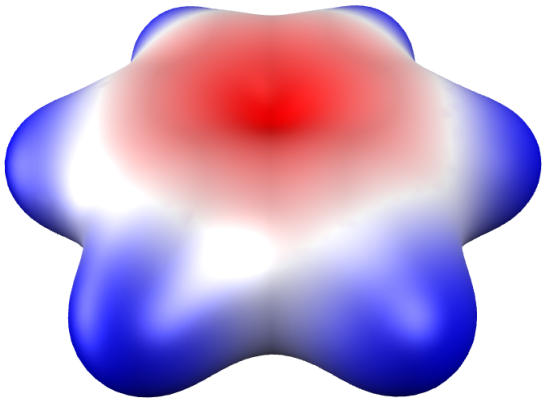
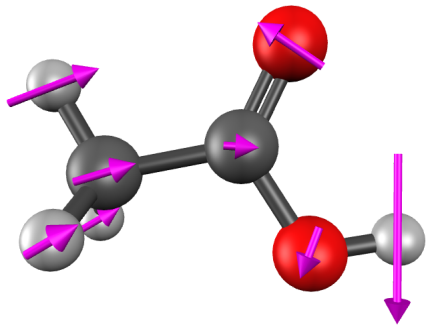


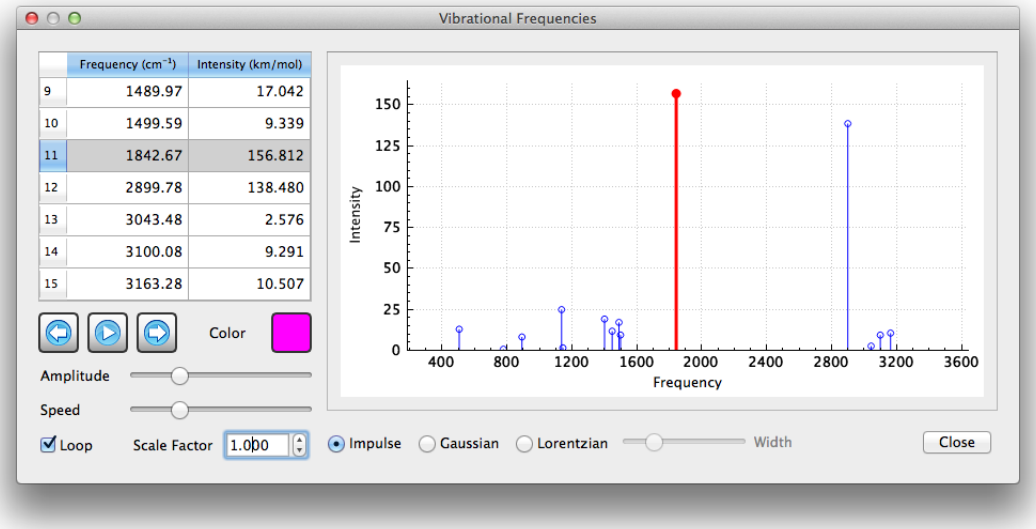
Figure 1: Electron density plot of benzene colored according to the electrostatic potential

4.3 Vibrational Frequencies

Vibrational frequencies can be read in from a Q-CHEM output file and appear as a Frequencies item in the MV. Normal mode vectors can be visualized by selecting the associated frequency item in the MV.



Double-clicking a frequency in the MV will cause the molecule to vibrate according to the selected mode. Double-clicking the Frequencies item will bring up the Vibrational Frequencies dialog:



This dialog contains an impulse spectrum showing the positions and relative intensities of the frequencies. Individual modes can be selected on the spectrum by clicking the hollow circles and this will also update the Viewer window with the selected mode. The impulses can be broadened using either Gaussians or Lorenzians to give a more realistic looking spectrum.

The horizontal scale of the spectrum can be zoomed (using the scroll wheel on the mouse) and translated (left-click and drag) to give greater detail.