Introduction to IQmol: Part I

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Resources

- Written by Dr. Andrew Gilbert
- Keep yourself up to date with IQmol
  website: http://iqmol.org

- IQmol Youtube channel: IQmol
  now has its own Youtube channel
Open IQmol, the molecule building screen looks like this:
Main build tools

Build Mode
Add Hydrogens
Minimize Energy (classical forcefield)

Build Elements
Add Fragments
(periodic table)
(pre-build molecules)
Click the “Build Element” : periodic table pops-up:
Select an atom, for example Oxygen: O
Click in the blue screen area to place the Oxygen atom
Add Hydrogen

- Click the “Add Hydrogens” button:
Click the “Minimize Energy” button to get a more realistic structure.

Energy of the current structure
Build —> Select Force Field: allows you to choose different force field

Classical minimizer
Pre-build molecule library (“Add Fragments” button) contains various molecules that can be used to build more complex molecules.
Click on the “Add Fragment” button, then choose `amino_acids/L-lysine`.
Click the “Add Fragment” button again, choosing the same molecule. Hold CTRL and the right mouse button (two fingers on Mac Trackpad) and drag the highlighted molecule – the screen should now look like this:
Click on the “Manipulate” mode

- Use left mouse button to rotate
- Use right mouse button to translate

<table>
<thead>
<tr>
<th>Rotation of all atoms: Left click + drag</th>
<th>Rotation of selected atoms: CTRL + left click + drag</th>
</tr>
</thead>
<tbody>
<tr>
<td>Translation of all atoms: R click + drag</td>
<td>Translation of selected atoms: CTRL + L click + drag</td>
</tr>
</tbody>
</table>
Select Mode

- Click on the “Select” mode

- Click on atoms to select them
- Click anywhere on the main window to deselect atoms
- Press “Alt” and the right mouse (two fingers on Mac Trackpad) button to move the group of selected atoms
Measuring bond length, angles, and dihedrals

- Click the select button
- Select 2, 3 or 4 atoms as necessary
- The measured bond length, angle or dihedral is displayed in the bottom corner:

The bond angle is displayed here
Performing Q-Chem calculations
Example 1: H$_2$O

Prerequisite: Consult IQmol-Server-Setup tutorial
• Build molecule, clean-up (force-field opt-n), check symmetry (symmetrize molecule)
• Optimize B3LYP/6-31G*
• Play with changing the view of the molecule, move it around, zoom
• Use ‘Select’ feature to measure bonds and angles
• Look at MOs: HOMO, HOMO-1; LUMO
• Run FREQ job, look at vibrations (click versus double-click)
Building up/Check symmetry
Performing Q-Chem

- Calculation —> Q-chem Setup; Open Q-chem User Interface (QUI) input editor
- QUI has 2 windows

Details of the calculation

Preview of the input file
There are 2 windows in “Computational details” section

- Basic setup
  - Label
  - Calculate: Energy
  - Exchange: HF
  - Correlation: None
  - Unrestricted
  - Max Cycles: 50
  - Convergence: 5

- Advanced calculations
  - Section: Job 1
  - Charge: 0
  - Multiplicity: 1
  - Basis: 6-31G
  - ECP: None
  - Second Basis: None
  - RI Basis: None
Setting up the job type, method, basis set
Setting up the job type, method, basis set
Setting up the job type, method, basis set
Take H$_2$O molecule and perform “Optimization” and “Frequency” analysis

First optimization:
Use add button to submit multiple jobs within one input file: such as optimization and frequency to be performed subsequently.

New job starts

Read the geometry from the previous calculation
- One can manually modify the input preview

- $\text{rem}$ section
Save the input on a disk: **File —> save as**

- Use `.inp` for name of the input file
Submitting job to HPC

Give a name and remember it.
- Use default queue on HPCC;
- Leave the rest of settings unchanged.

**For advanced users:**
- To run Q-Chem in parallel (openmp), change the number in CPUs (**consult the manual** to see which types of jobs are openmp-parallelized);
- for MPI-parallel, you will need to tweak the settings in the previous page;
- Memory and scratch settings are not important here, but for optimal performance you may need to tweak these settings in the Q-Chem input file, especially for advanced calculations. **Consult the manual** before doing so!
Check the job status by selecting: “Calculation —>Job Monitor”
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<table>
<thead>
<tr>
<th>Job</th>
<th>Server</th>
<th>Submit Time</th>
<th>Run Time</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Educt-OptFreq</td>
<td>fluffy</td>
<td>14:28:24</td>
<td></td>
<td>Queued</td>
</tr>
<tr>
<td>Product-OptFreq</td>
<td>fluffy</td>
<td>14:44:54</td>
<td></td>
<td>Queued</td>
</tr>
<tr>
<td>TS-OotFreq</td>
<td>fluffy</td>
<td>14:49:47</td>
<td></td>
<td>Queued</td>
</tr>
<tr>
<td>CH2O</td>
<td>hpc</td>
<td>18:08:04</td>
<td>0:02:34</td>
<td>Finished</td>
</tr>
<tr>
<td>CH2O-NBO</td>
<td>hpc</td>
<td>18:30:56</td>
<td>0:00:06</td>
<td>Finished</td>
</tr>
<tr>
<td>H2O</td>
<td>hpc</td>
<td>15:19:35</td>
<td></td>
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Job status is displayed in a new window:

- Use left mouse button to select the job
- Use right mouse button to see this menu
- Kill the job by selecting this option
Job is finished
Copy files to your laptop

Note:
Must be the same name as the folder you have created while submitting the job

If they do not match, you will get “no valid data found in …” error message. The files are actually OK and are copied to your laptop. You can open them individually with “Open…” command.
After you copied files to your laptop

Golden star shows that it is copied properly

Click the checkbox!
After the calculations have completed, open the .out (output) with iQmol. The example here is H$_2$O after optimization and frequency analysis.

Click the small arrow next to the checkbox to see various calculated properties.

Clicking the arrow next to **Geometries** gives the calculated energy at every step of optimization.
Clicking the arrow next to **Frequencies** gives the calculated frequencies and displaced vectors for each frequency (for H\textsubscript{2}O: 3N-6=3 vibrational frequencies)

Double click at each value to animate the vibration
Must add GUI = 2 in the $ rem section (IQmol does it by default)

Open .Fchk file to see orbitals, density, spin density and so on.

Click at Surfaces and a window pops-up
Select orbital
Select the relevant orbital (default: HOMO)
Select the quality you want
Click calculate

click the arrow next to **Surfaces** to see the orbitals one by one by clicking the checkbox of the corresponding orbital (do not forget to uncheck the old one)
Use “Manipulation” mode to better see the orbital

To save the screen: **File —> Save Picture**
Select different properties to be calculated; spin density, density, and so on....
Performing Q-Chem calculations

Example 2: CH$_2$O (Formaldehyde)
• Build molecule, clean-up (force-field opt-n), check symmetry (symmetrize molecule)
• Optimize wB97X-D/6-31+G*
• Play with changing the view of the molecule, move it around, zoom
• Use ‘Select’ feature to measure bonds and angles
• Look at MOs: HOMO, HOMO-1, LUMO
• Run FREQ job, look at vibrations (click versus double-click)
• Advanced: Run NBO analysis, look at NBO charges and bond orders
Building up/Check symmetry
CH$_2$O Optimization
Submitting job to HPC
Choosing queue
Monitoring submitted job
**Monitoring submitted job**

![Process Monitor](image)

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Job is finished
Copy files to your laptop

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Analyze the output

click checkbox
Optimization cycles
3N-6 = 6 vibrational frequency
Use “Select” mode to choose a bond, angle, torsion, …
- **Must add GUI = 2 in the $ rem section** (IQmol does it by default)
- Open `.Fchk` file to see Orbitals, Density, Spin density and so on.
- Click at **Surfaces** and a window will pops-up
Select Orbital
Select the relevant orbital (default: HOMO)
Select the quality you want
Click calculate

Click the arrow next to **Surfaces** to see the orbitals one by one by clicking the checkbox of the corresponding orbital (do not forget to uncheck the old one)
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