Introduction to IQmol: Part I

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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:
Iqmol: Quick overview

Model View (MV)  Tool Bar

History  Viewer

Q-CHEM A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY
IQmol: Main build tools

Build Mode

Add Hydrogens

Minimize Energy (classical forcefield)

Build Elements (periodic table)

Add Fragments (pre-built molecules)
Click the “Build Element”: periodic table pops up:
IQmol: Selecting atom

- Select an atom, for example Oxygen: O
- Click in the blue screen (Viewer) area to place the Oxygen atom
Click the “Add Hydrogens” button:
Click the “Minimize Energy” button to get a more realistic structure.
IQmol: Classical minimizer

- Build —> Select Force Field: allows you to choose different force field
IQmol: Pre-build molecules

- 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 on the “Manipulate” mode.

Activating this mode changes the cursor to 🖐️. This is the default mode for the viewer and allows the molecule to be rotated and zoomed.

The manipulate mode implements the following mouse functions:

- **Left click and drag**: Rotate the view of the molecule. Cursor changes to 🖐️
- **Middle click and drag**: Zoom in and out. Cursor changes to 🕵️
- **Right click and drag**: Translate the view of the molecule. Cursor changes to 🏞️

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

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

Replace CTRL with command key for Mac.
IQmol: Select Mode

- Click on the “Select” mode

Activating this mode changes the cursor to $\text{Select}$. This mode can also be activated using the $\text{shift key}$ when in manipulate mode.

The select mode 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.

- Press “CTRL” and the left/right mouse (two fingers on Mac Trackpad) button to move the group of selected atoms [Replace CTRL with command key for Mac. For Mac Tracpad do the corresponding finger gesture]
IQmol: Measuring bond length, angles, and dihedrals

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

The bond length 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 Calculations

From menu bar:

- 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.
Setting up the job type, method, basis set
Setting up the job type, method, basis set

<table>
<thead>
<tr>
<th>Job Section</th>
<th>Job 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculate</td>
<td>Energy</td>
</tr>
<tr>
<td>Method</td>
<td>HF</td>
</tr>
<tr>
<td>Basis</td>
<td>HF</td>
</tr>
<tr>
<td>Exchange</td>
<td>B3LYP</td>
</tr>
<tr>
<td>SCF Control</td>
<td>B3LYP</td>
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<tr>
<td>Charge</td>
<td>0</td>
</tr>
<tr>
<td>Multiplicity</td>
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<tr>
<td>ECP</td>
<td>None</td>
</tr>
<tr>
<td>Correlation</td>
<td>None</td>
</tr>
</tbody>
</table>
Setting up the job type, method, basis set

![Image of Q-Chem interface showing job setup options for energy calculation, method (HF), basis set (6-31G), and exchange (3-21G), with advanced options for SCF controller, algorithm, and max cycles.]
- 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
Input editing

- One can manually modify the input preview

- $rem$ section
- Save the input on a disk: File ➔ save as
- Use .inp for name of the input file
Give a name and remember it.

Submitting job to Iqmol server 
iqmol.q-chem.com
Check the job status by selecting: “Calculation —> Job Monitor”
Check the job status by selecting: “**Calculation —>Job Monitor**”
Monitoring submitted job

- Job status:
  - 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

Create new folder to store output files:

![Image of folder creation dialog in IQmol software]
After you copied files to your laptop

Golden star shows that it is copied properly.

Click the checkbox!
Analyzing Output: Optimization

- After the calculations has been completed, open the .out (output) with IQmol. The example here is H₂O 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$_2$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.
- Double click on **MO Surfaces** under **Molecular Orbitals** (mac) and a window pops up
- For MS Windows views are little different
- Just double click on **MO Surfaces** and “Add Surface” window pops up
Select orbital
Select the relevant orbital (default: HOMO)
Select the quality you want
Click calculate

Click the arrow next to **MO 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 “Manipulate Mode” to better see the orbital
To save the screen: File —> Save Picture
To change the quality of the surface double click on the orbital being displayed in MV.
- Double click on **MO Surface** again from MV panel
- “Add Surface” window will pop up again
- 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
CH$_2$O Frequency
Submitting job to QChem
Monitoring submitted job
### Monitoring submitted job

<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>Cr2O7_dichromate</td>
<td>QChem</td>
<td>16:25:39</td>
<td>0:03:27</td>
<td>Finished</td>
</tr>
<tr>
<td>H2O</td>
<td>QChem</td>
<td>22:08:49</td>
<td>0:01:57</td>
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<tr>
<td>CH2O</td>
<td>QChem</td>
<td>11:20:08</td>
<td>0:00:20</td>
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<tr>
<td>CH2O</td>
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<td>11:23:59</td>
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<td>CH2O</td>
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<td>11:25:04</td>
<td></td>
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<tr>
<td>CH2O</td>
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<td>11:26:25</td>
<td></td>
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<tr>
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<td>11:26:56</td>
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<tr>
<td>CH2O</td>
<td>QChem</td>
<td>11:28:03</td>
<td></td>
<td>Queue</td>
</tr>
</tbody>
</table>

**Clear List**

**Close**
Job is finished
Copy files to your laptop

```
<table>
<thead>
<tr>
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<th>Run Time</th>
<th>Status</th>
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</thead>
<tbody>
<tr>
<td>31</td>
<td>Cr2O7 dichromate</td>
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<td>Finished</td>
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<tr>
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<td>QChem</td>
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<td>Finished</td>
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<tr>
<td>38</td>
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<td>QChem</td>
<td>11:28:03</td>
<td>0:00:08</td>
<td>Finished</td>
</tr>
</tbody>
</table>
```
Analyze the output

click checkbox
Optimization cycles
3N-6= 6 vibrational frequency
Measuring parameters

- Use “Select” mode to choose a bond, angle, torsion, …
HOMO-LOMO orbitals

- 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 MO Surfaces and a window will pop 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**