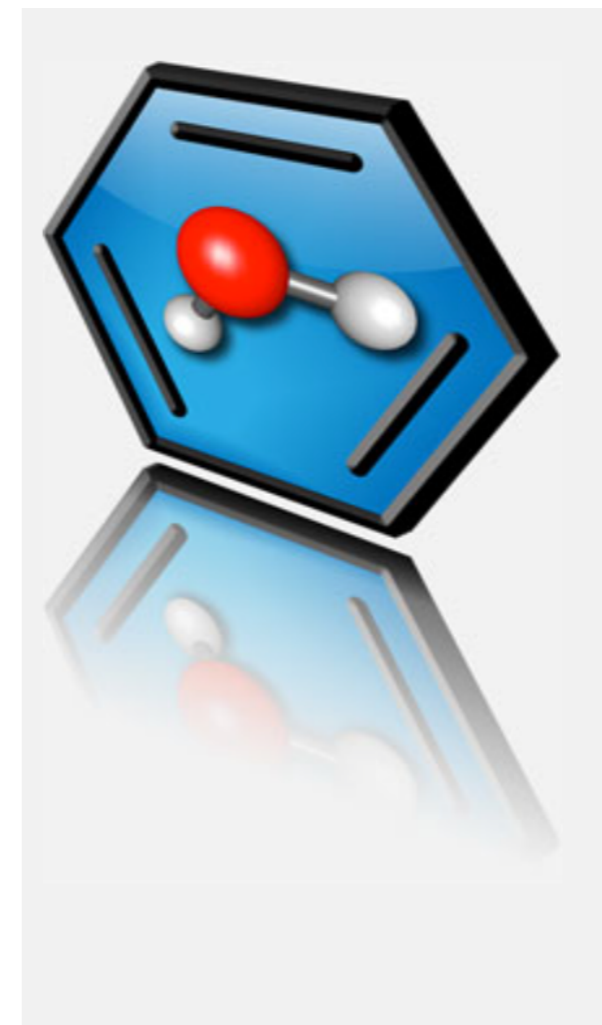


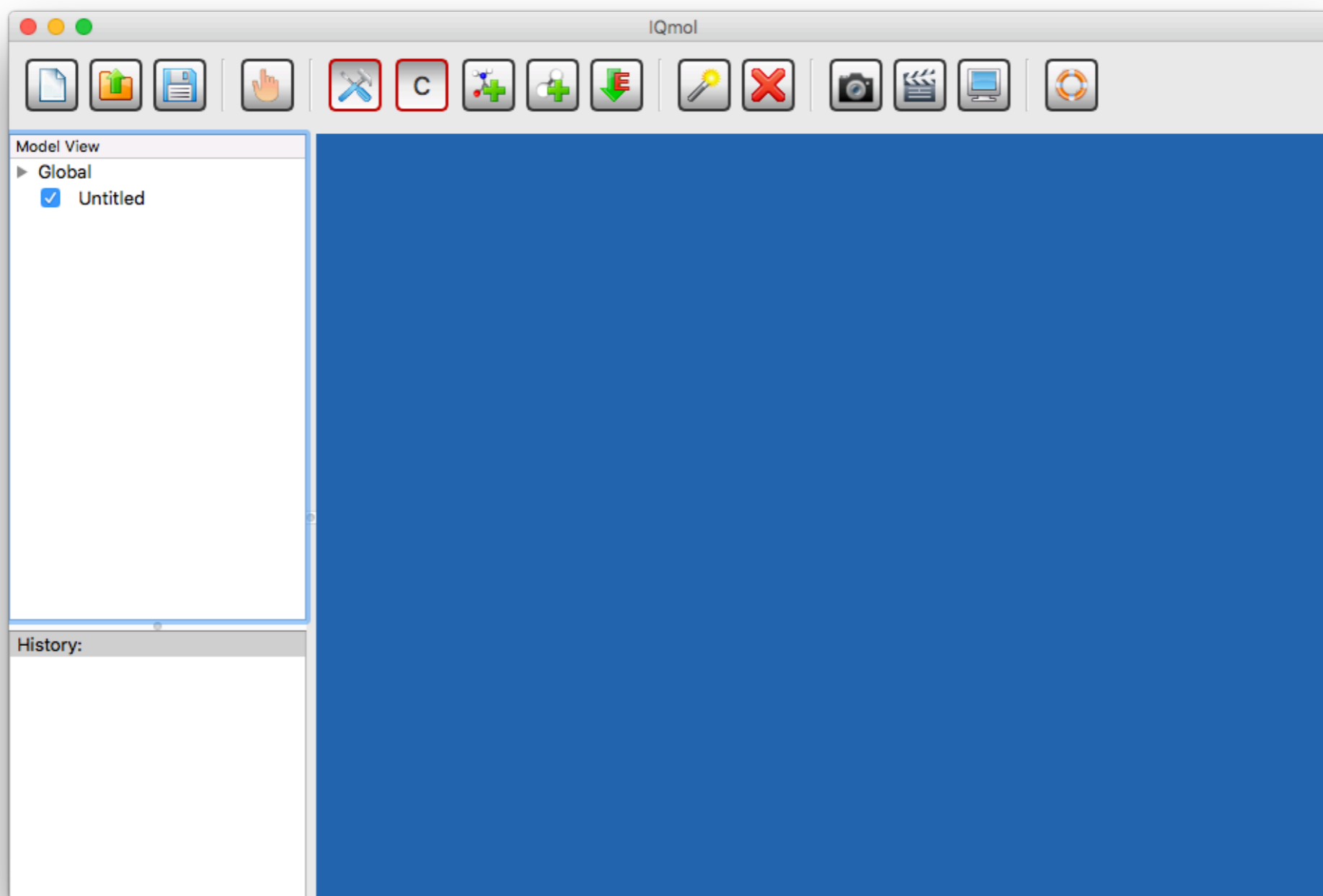
Introduction to IQmol: Part I

Fazle Rob, Shirin Faraji, Ilya Kaliman, and Anna Krylov

- 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:



Model View (MV) **Tool Bar**

Model View

- Global
- [-] Untitle
- [-] Atoms
 - C1
 - C2
 - H3
 - H4
 - H5
 - H6
 - H7
 - H8
- Bonds

History:

- Add atoms/bonds
- Add hydrogens
- Minimize energy

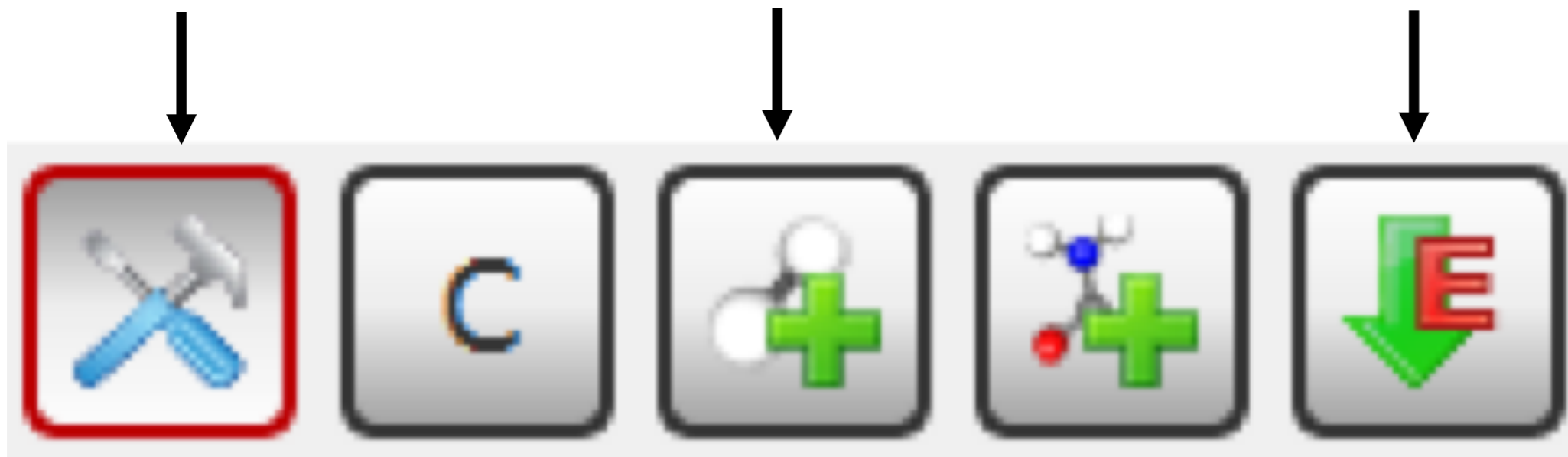
UFF energy: 0.5888

History **Viewer**

Build Mode

Add Hydrogens

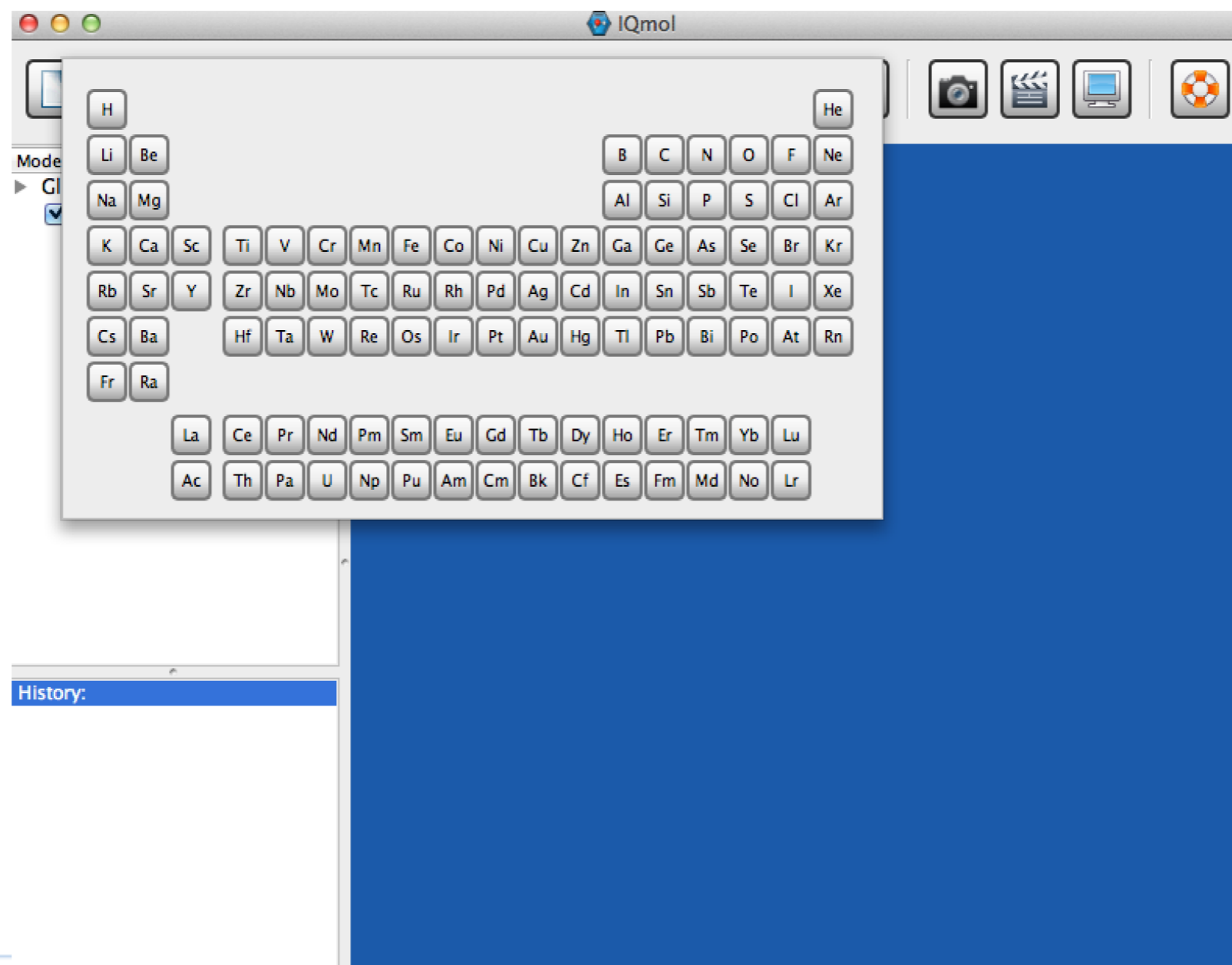
Minimize Energy (classical forcefield)



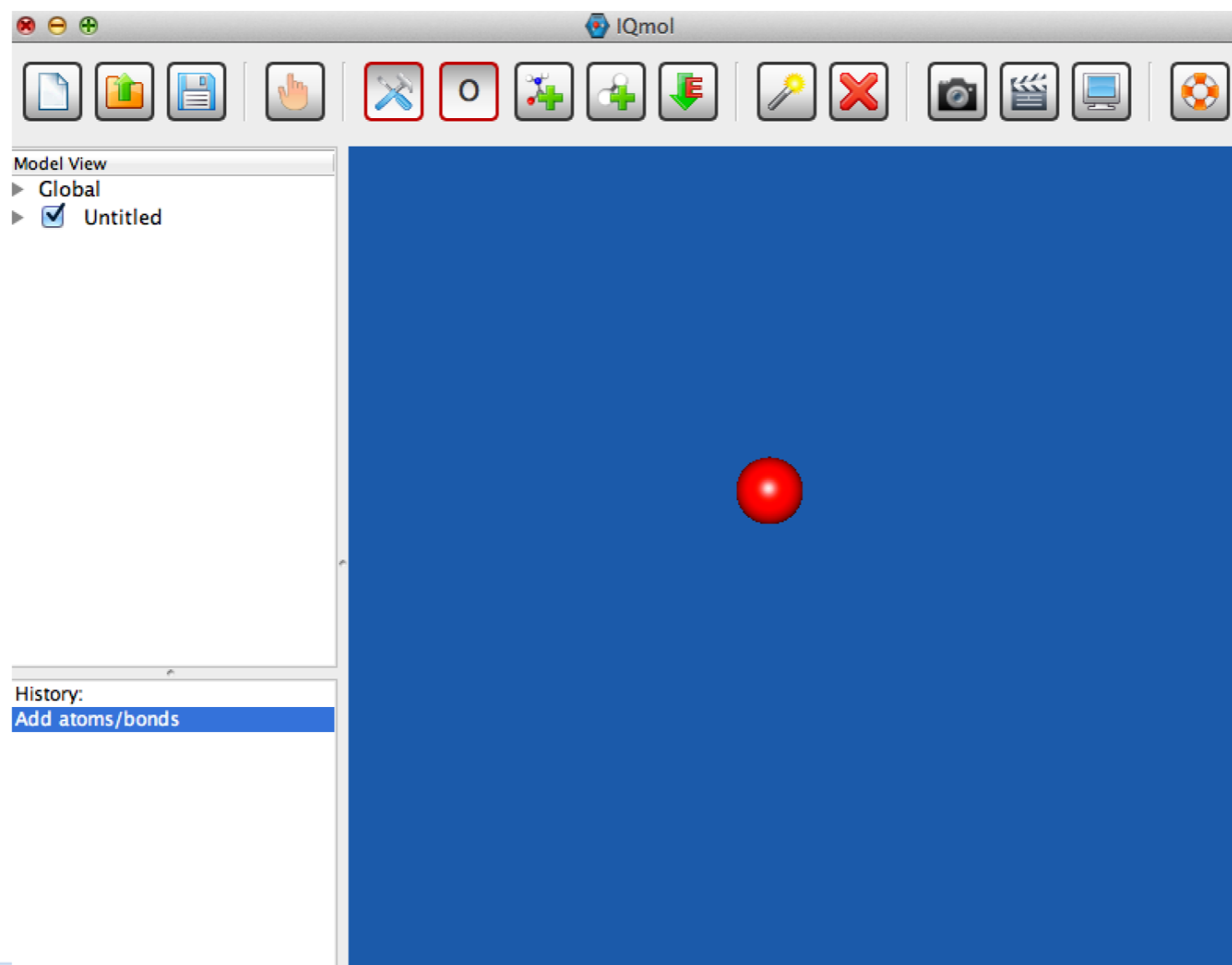
Build Elements
(periodic table)

Add Fragments
(pre-built molecules)

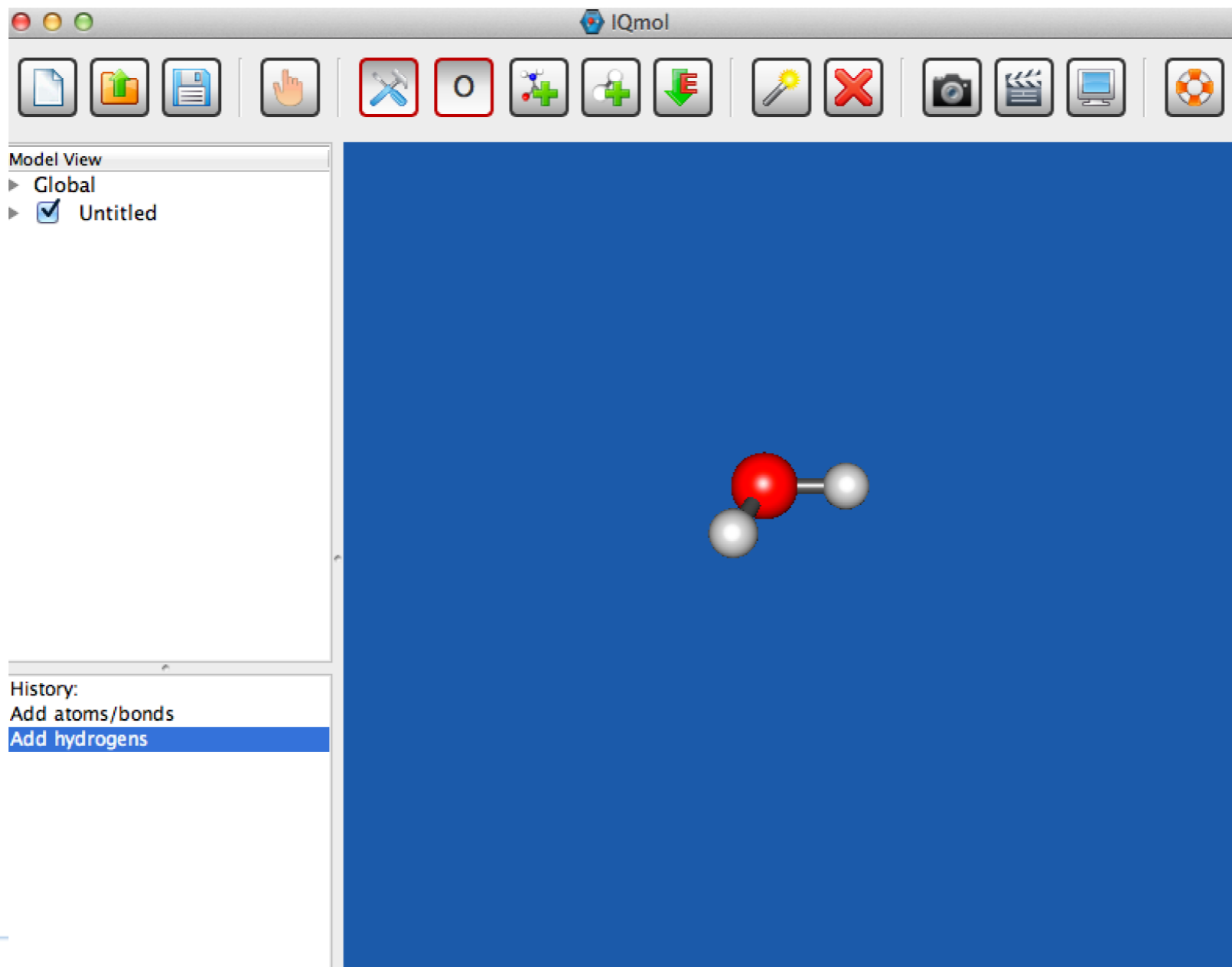
- Click the “Build Element” : periodic table pops up:



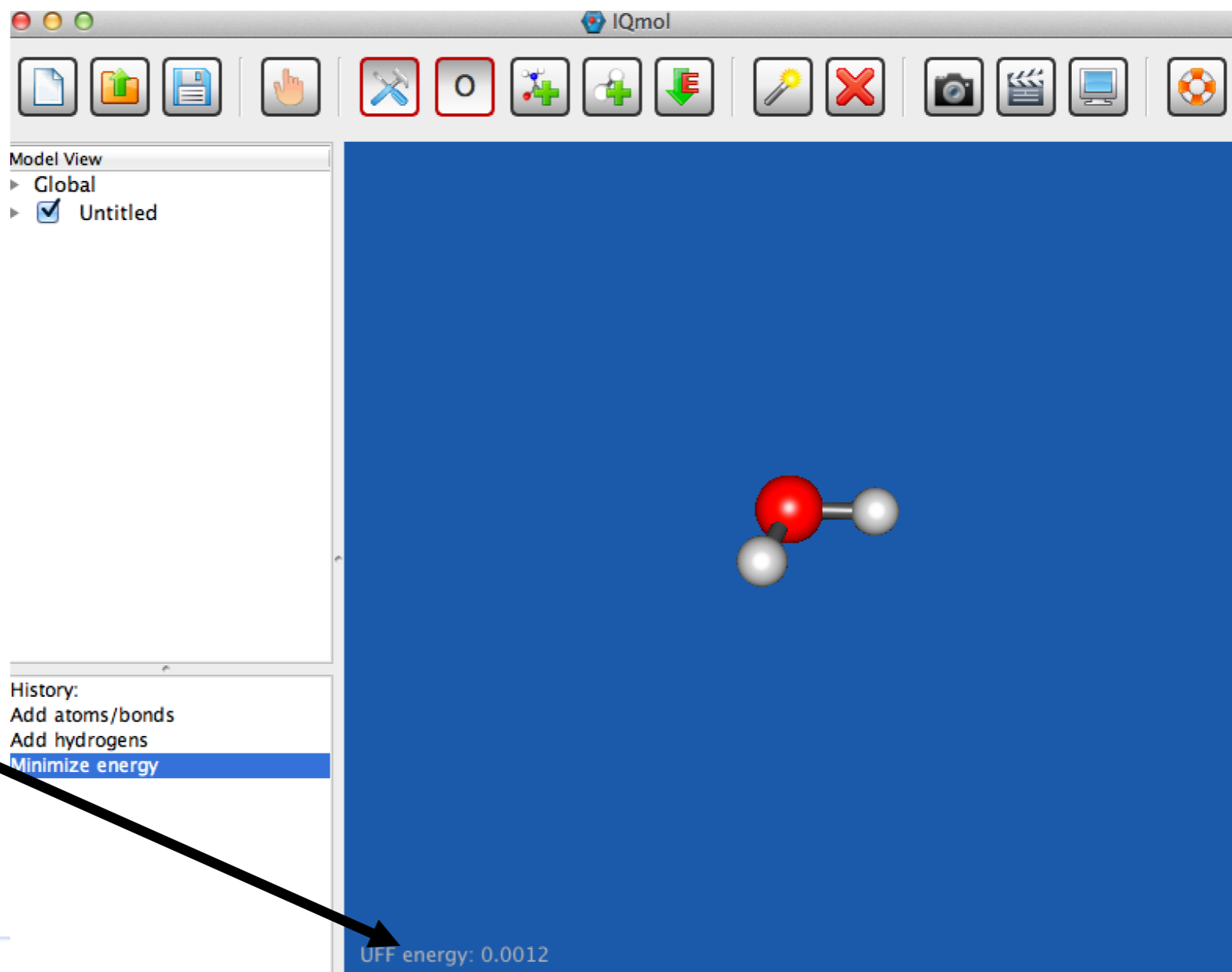
- Select an atom, for example Oxygen: O
- Click in the blue screen (Viewer) area to place the Oxygen atom



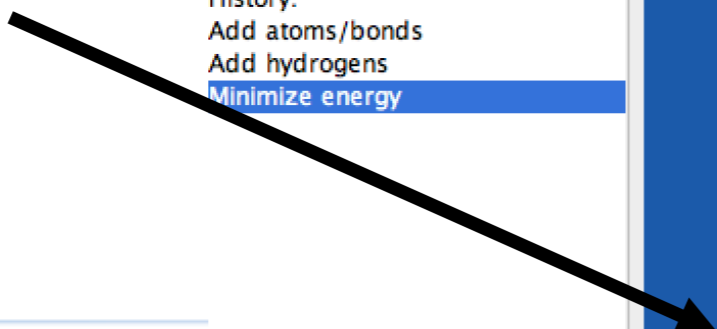
- Click the “Add Hydrogens” button:



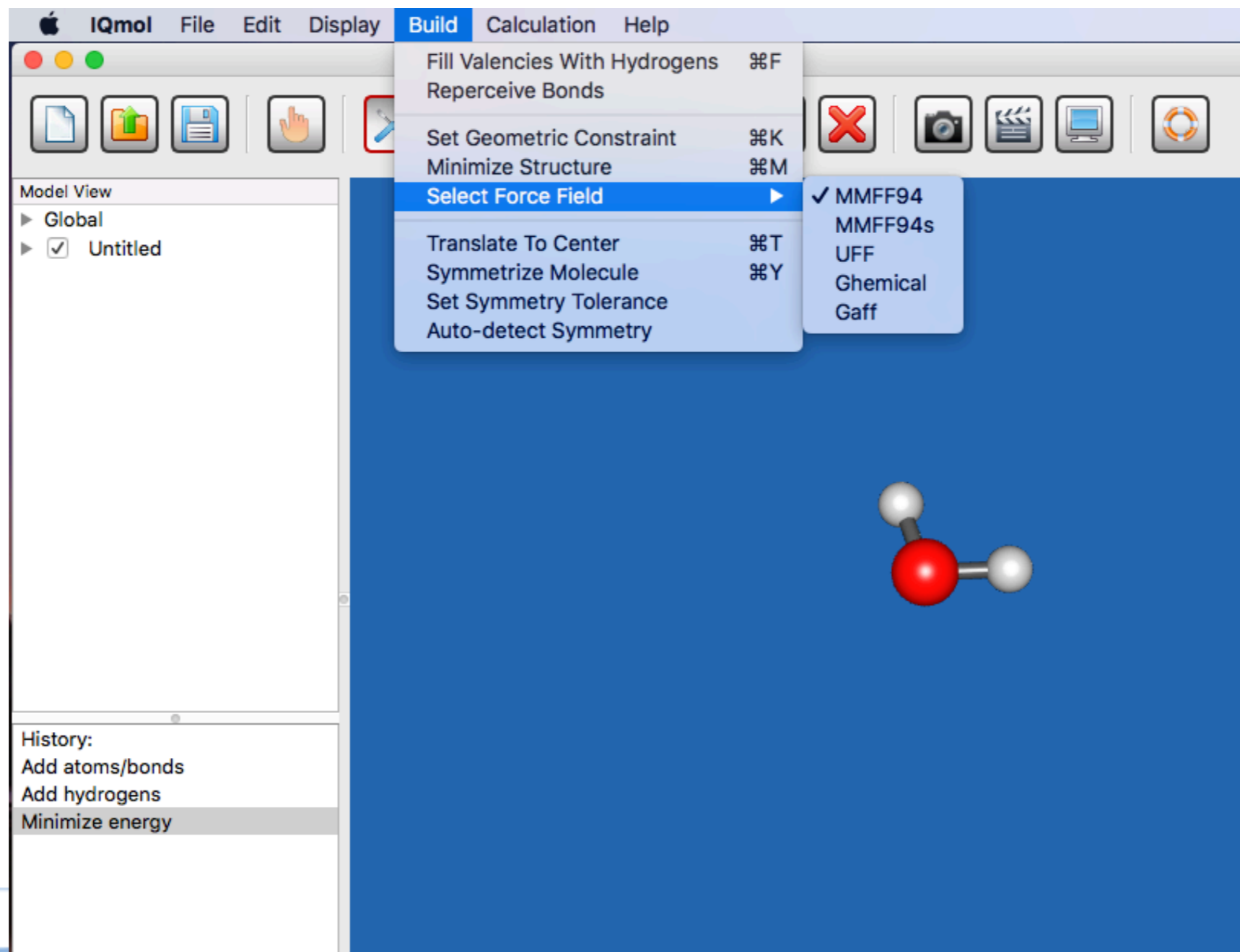
- Click the “Minimize Energy” button to get a more realistic structure



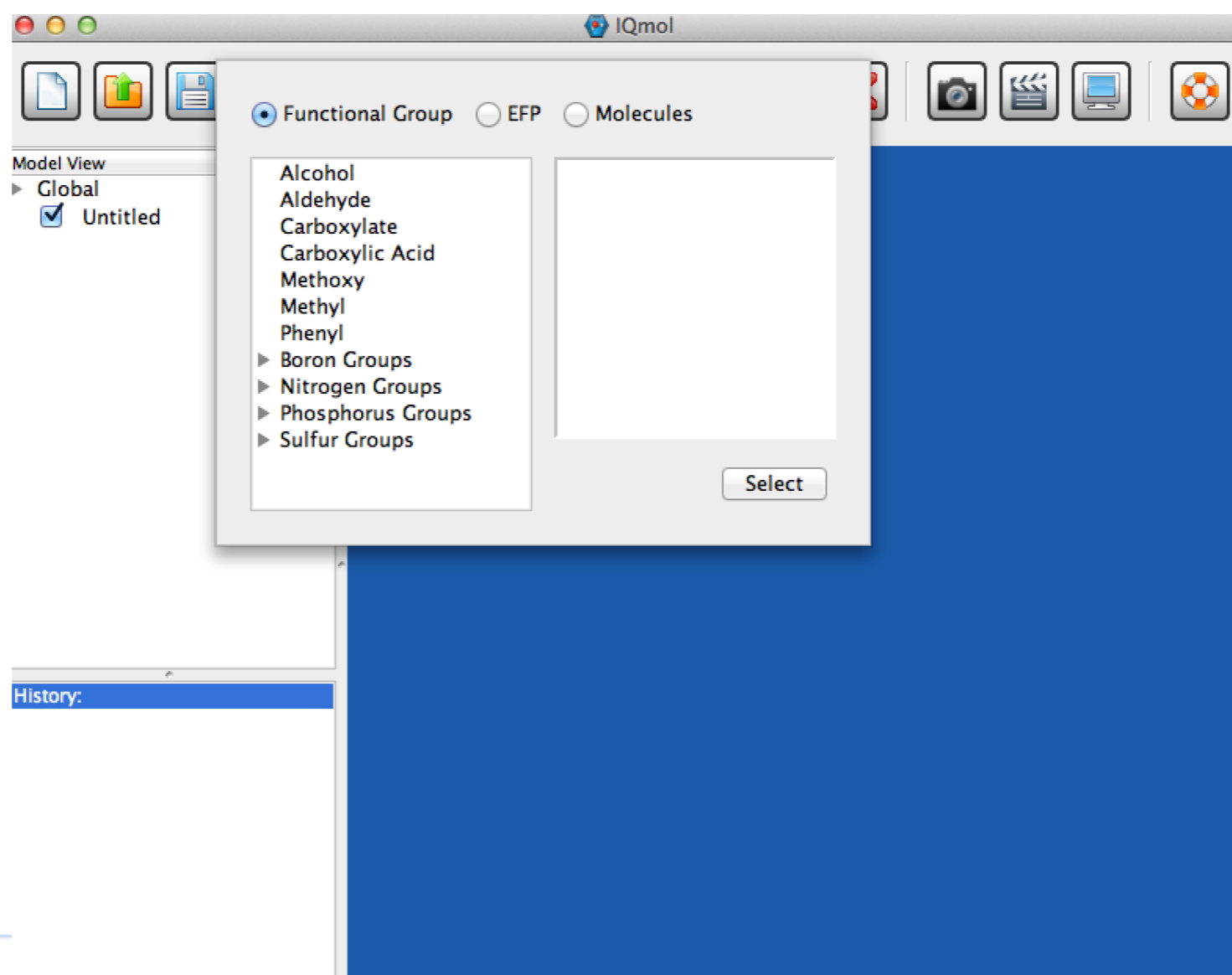
Energy of the current structure



- Build → Select Force Field: allows you to choose different force field



- 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.




The screenshot displays the IQmol software interface. A dialog box titled 'Add Fragment' is open, showing three radio buttons: 'Functional Group', 'EFP', and 'Molecules' (which is selected). Below these buttons is a list of amino acids: L-Arginine, L-Asparagine, L-Aspartic acid, L-Cysteine, L-Glutamic acid, L-Glutamine, L-Histidine, L-Isoleucine, L-Leucine, L-Lysine (highlighted in blue), L-Methionine, L-Phenylalanine, and L-Proline. To the right of the list is a chemical structure of L-lysine, showing a six-membered ring with two amino groups (H₂N) and a carboxylic acid group (COOH). A 'Select' button is located at the bottom right of the dialog box. In the background, the main interface shows a 'Model View' panel with 'Global' and 'Untitled' (checked) options, and a 'History' panel with 'Add molecule' listed.

- 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 

Rotation of all atoms: Left click + drag

Rotation of selected atoms: CTRL + left click + drag


Translation of all atoms: R click + drag

Translation of selected atoms: CTRL + L click + drag

Replace CTRL with command key for Mac

- Click on the “Select” mode




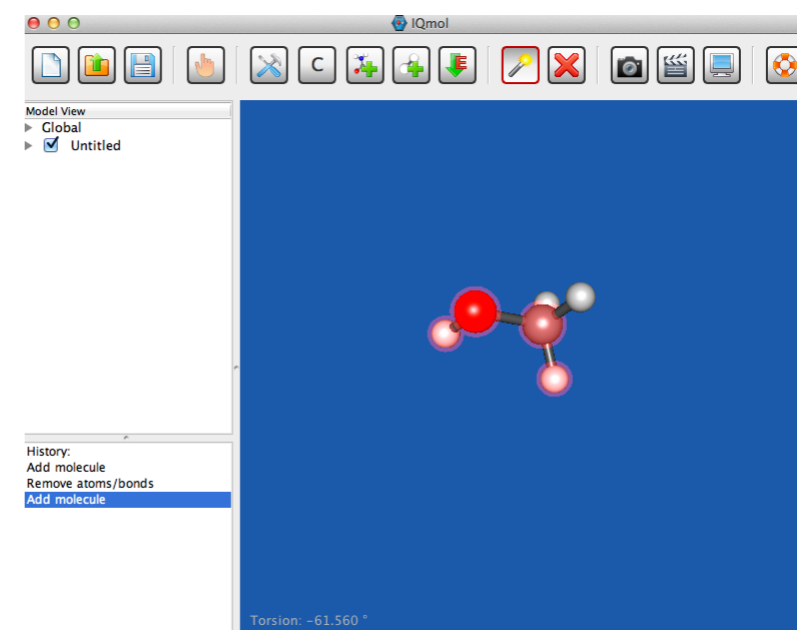
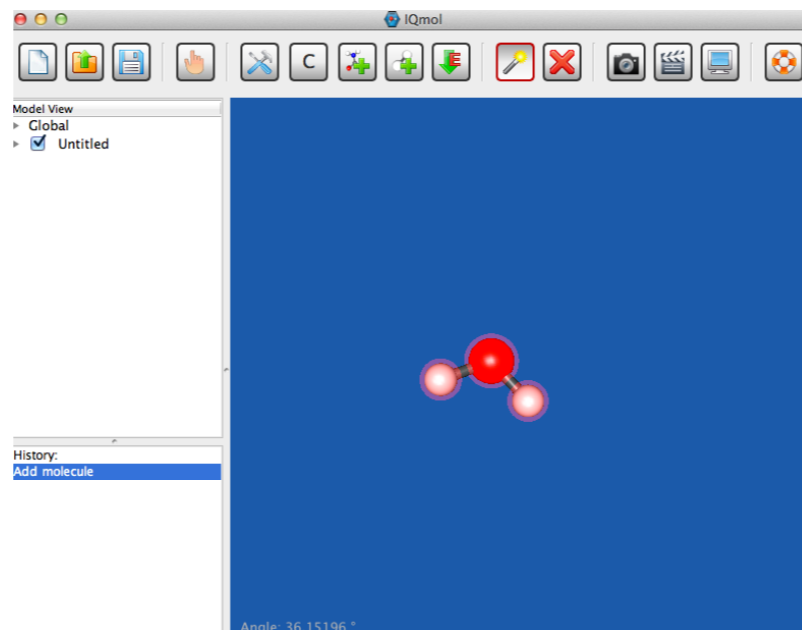
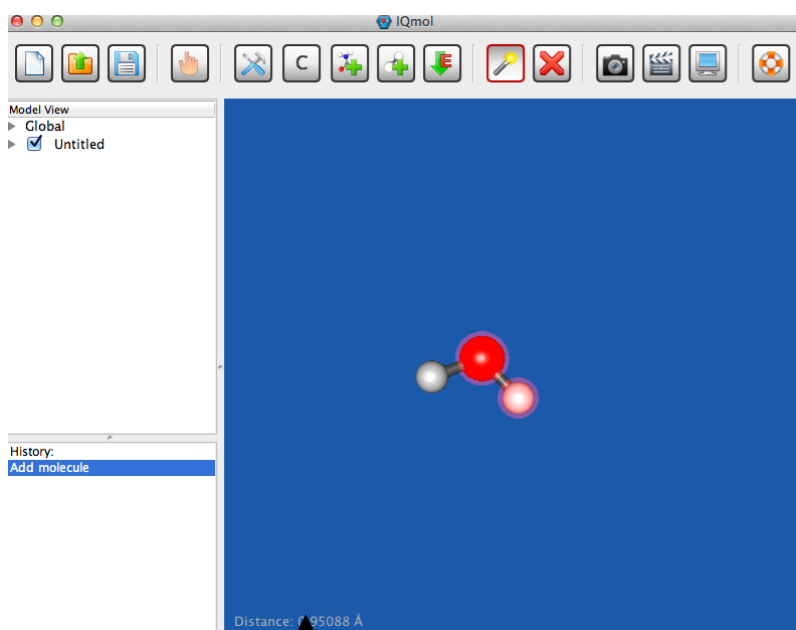
Activating this mode changes the cursor to . This mode can also be activated using the *shift key* when in manipulate mode.

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**]

- 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: H₂O

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

The image displays two side-by-side screenshots of the IQmol software interface, illustrating the process of symmetrizing a molecule.

Left Screenshot: Shows the initial structure of a water molecule (H₂O). The history panel lists: Add atoms/bonds, Add hydrogens, and Minimize energy. The UFF energy is 0.0000.

Right Screenshot: Shows the 'Build' menu open, with 'Symmetrize Molecule' selected. The history panel is updated to include 'Symmetrize structure'. The point group is identified as C_{2v}.

Arrows point to the history panels in both screenshots, highlighting the changes in the workflow.

From menu bar: File Edit Display Build Calculation Help

- **Calculation** → **Q-chem Setup**; open Q-chem User Interface (QUI) input editor

IQmol

Setup Advanced

Job Section Job 1 Edit + -

Calculate Energy Charge 0

Method HF Multiplicity 1

Basis 6-31G ECP None

Exchange HF Correlation None

SCF Control

Algorithm DIIS Convergence 5

Guess SAD Max Cycles 50

Second Basis None Guess Mix 0%

Dual Basis Energy Unrestricted

Wavefunction Analysis

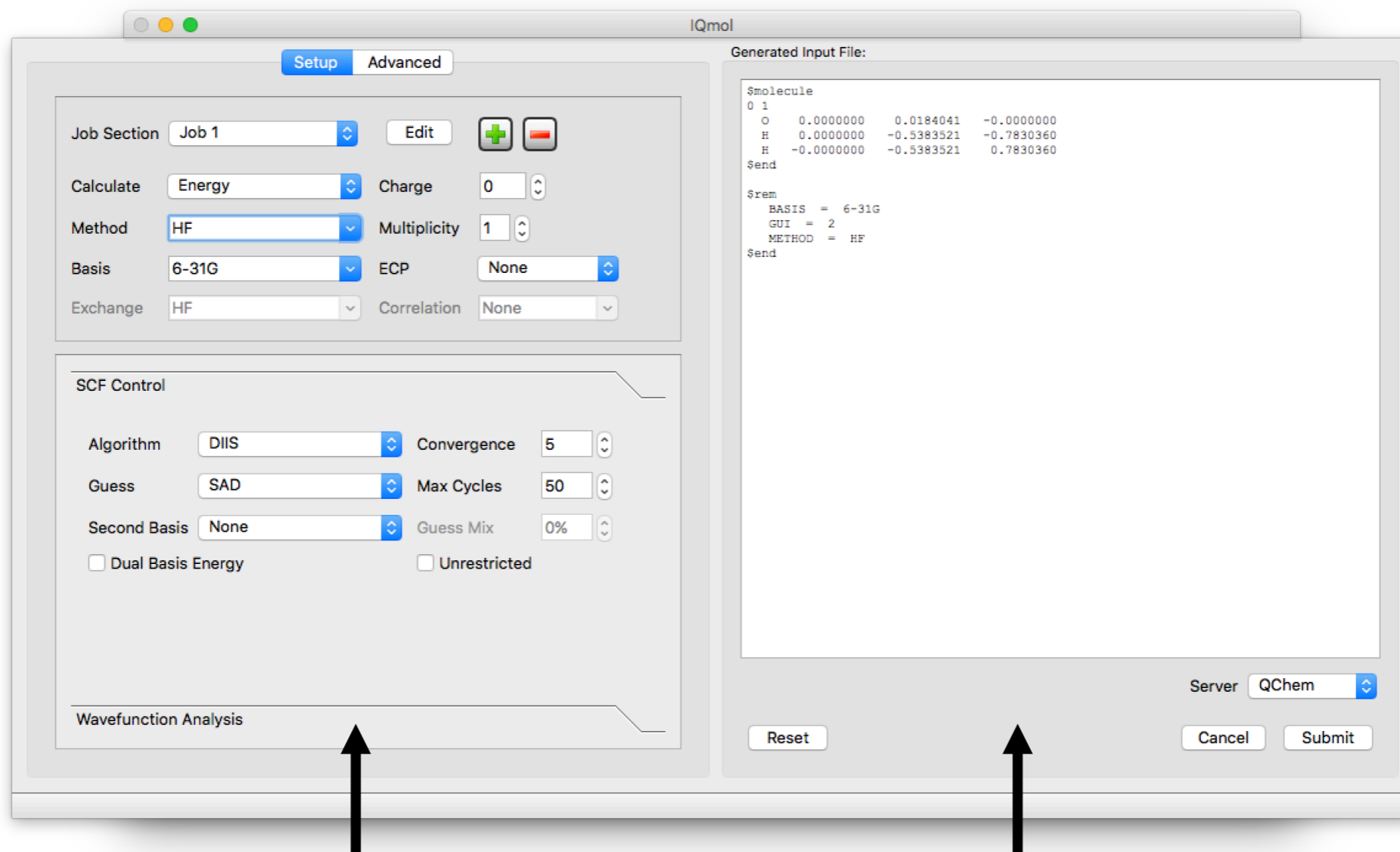
Generated Input File:

```
$molecule
0 1
O 0.0000000 0.0184041 -0.0000000
H 0.0000000 -0.5383521 -0.7830360
H -0.0000000 -0.5383521 0.7830360
$end
$rem
BASIS = 6-31G
GUI = 2
METHOD = HF
$end
```

Server QChem

Reset Cancel Submit

- QUI has 2 windows



Details of the calculation

Preview of the input file

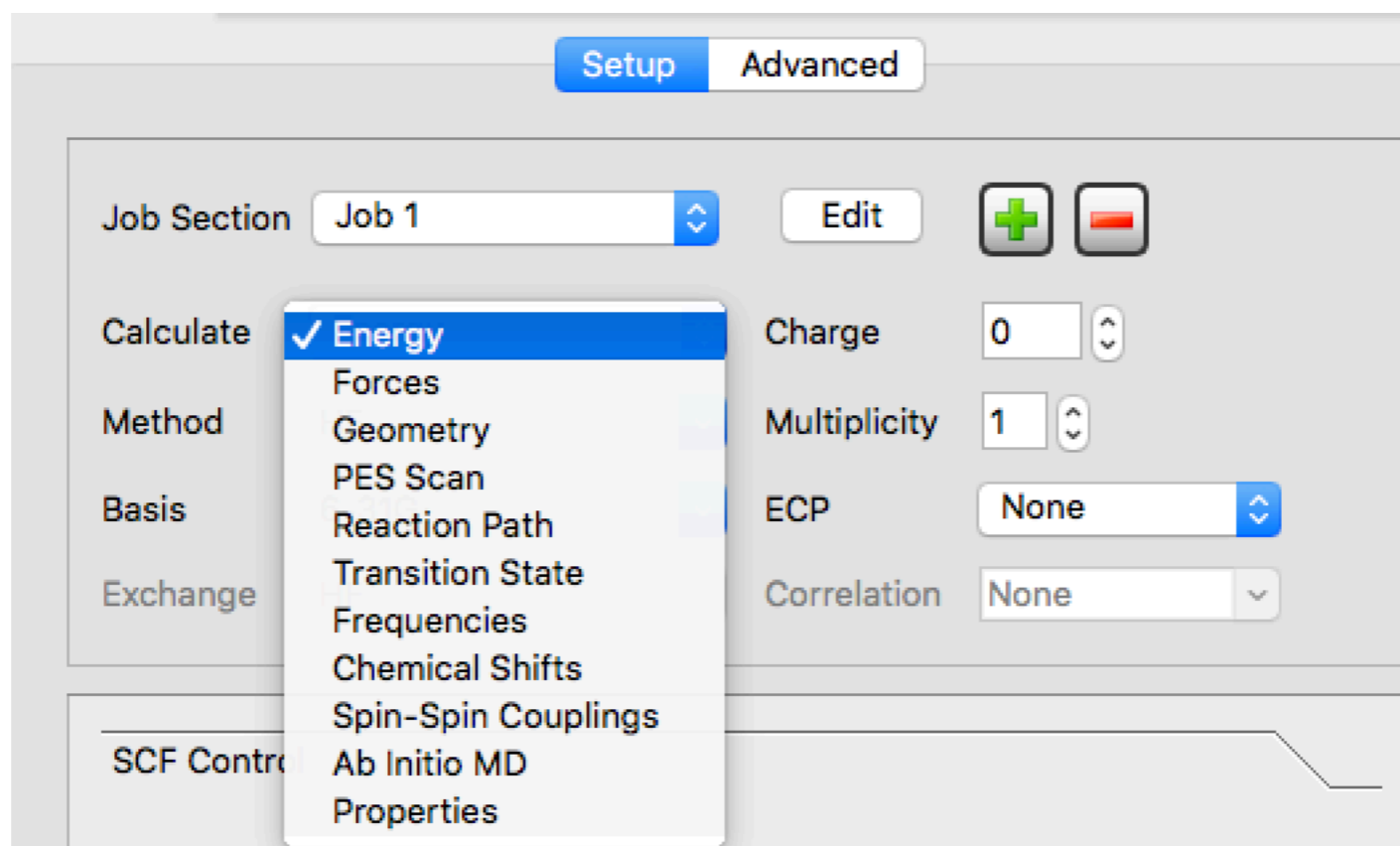
- There are 2 windows in “Computational details” section

Advanced calculations

Basic setup

The screenshot displays the 'Computational details' section of the Q-CHEM QUI interface. At the top, there are two tabs: 'Setup' and 'Advanced'. An arrow labeled 'Basic setup' points to the 'Setup' tab, and another arrow labeled 'Advanced calculations' points to the 'Advanced' tab. The 'Setup' tab is currently selected and contains the following configuration options:

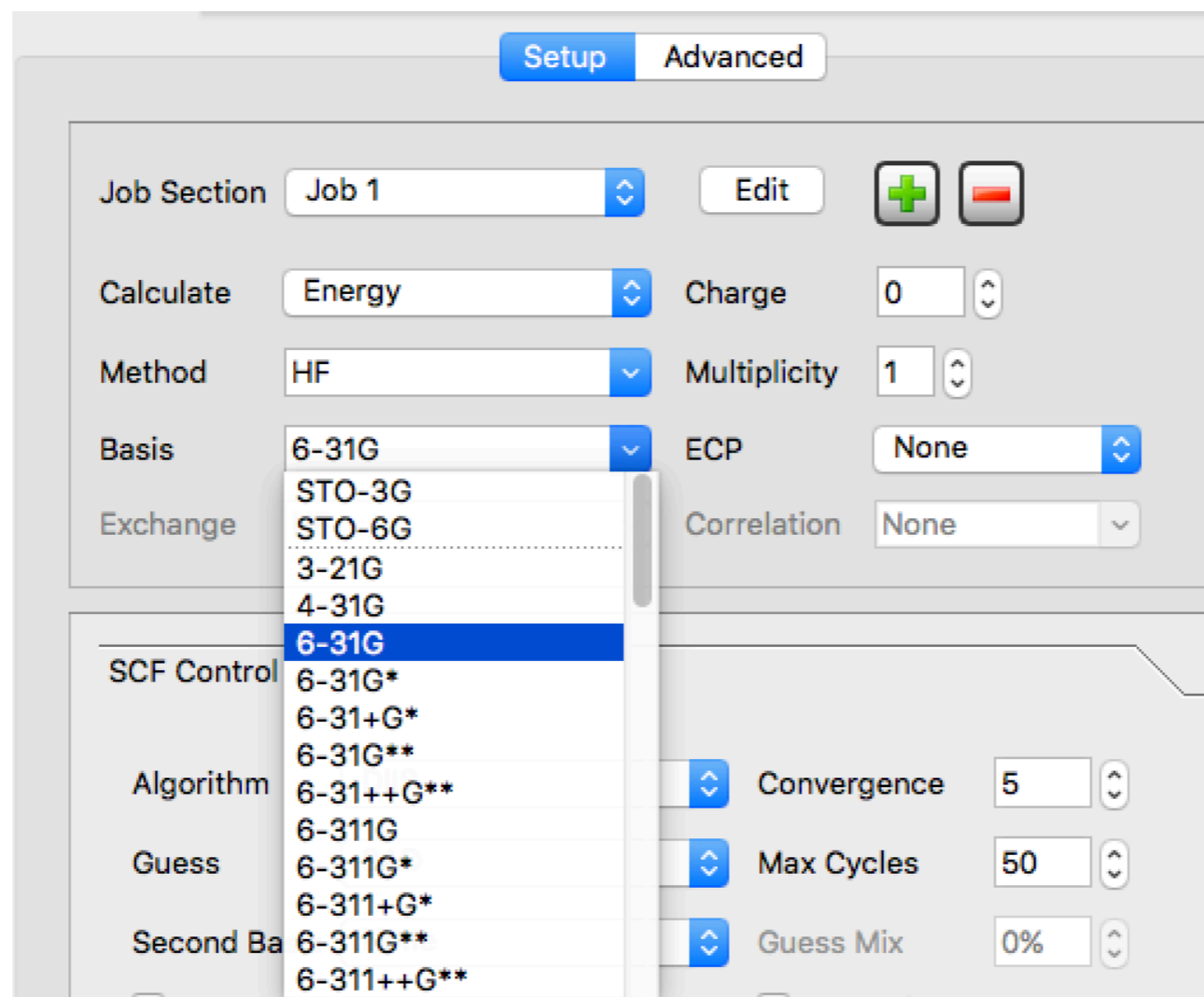
Job Section	Job 1	Edit	+ -
Calculate	Energy	Charge	0
Method	HF	Multiplicity	1
Basis	6-31G	ECP	None
Exchange	HF	Correlation	None



The screenshot displays the 'Setup' tab of the Q-Chem software interface. The 'Job Section' is set to 'Job 1'. The 'Calculate' option is 'Energy'. The 'Method' dropdown is open, showing a list of options: HF (highlighted), Custom, B3LYP, M06-2X, Omega-B97X-D, Omega-B97X-V, BLYP, CAM-B3LYP, and EDF1. The 'Basis' dropdown is set to 'None'. The 'Exchange' dropdown is set to 'None'. The 'SCF Control' dropdown is set to 'None'. The 'Charge' is set to 0, and the 'Multiplicity' is set to 1. There are also 'Edit', '+', and '-' buttons for job management.

Field	Value
Job Section	Job 1
Calculate	Energy
Method	HF
Basis	None
Exchange	None
SCF Control	None
Charge	0
Multiplicity	1
ECP	None
Correlation	None

Setting up the job type, method, basis set



The screenshot displays the 'Setup' tab of the Q-CHEM software interface. The 'Advanced' sub-tab is active. The 'Job Section' is set to 'Job 1'. The 'Calculate' dropdown is set to 'Energy', 'Charge' is 0, 'Multiplicity' is 1, 'ECP' is 'None', and 'Correlation' is 'None'. The 'Method' is set to 'HF'. The 'Basis' dropdown menu is open, showing a list of basis sets: 6-31G, STO-3G, STO-6G, 3-21G, 4-31G, 6-31G (highlighted), 6-31G*, 6-31+G*, 6-31G**, 6-31++G**, 6-311G, 6-311G*, 6-311+G*, 6-311G**, and 6-311++G**. The 'Exchange' dropdown is also open, showing the same list of basis sets. The 'SCF Control' section is visible, with 'Algorithm' set to '6-31++G**', 'Convergence' set to 5, 'Max Cycles' set to 50, and 'Guess Mix' set to 0%.

- Take H₂O molecule and perform “Optimization” and “Frequency” analysis
- First optimization:

Setup Advanced

Job Section: Job 1 Edit + -

Calculate: Geometry Charge: 0

Method: B3LYP Multiplicity: 1

Basis: 6-31G* ECP: None

Exchange: HF Correlation: None

SCF Control

Algorithm: DIIS Convergence: 8

Guess: SAD Max Cycles: 50

Second Basis: None Guess Mix: 0%

Dual Basis Energy Unrestricted

Wavefunction Analysis

Generated Input File:

```

$molecule
0 1
O 0.0000000 0.0184041 -0.0000000
H 0.0000000 -0.5383521 -0.7830360
H -0.0000000 -0.5383521 0.7830360
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Optimization
METHOD = B3LYP
SCF_CONVERGENCE = 8
$end

```

Server: QChem

Reset Cancel Submit

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



Setup | Advanced

Job Section: Job 2 [Edit] [Add] [Remove]

Calculate: Frequencies Charge: 0

Method: B3LYP Multiplicity: 1

Basis: 6-31G* ECP: None

Exchange: HF Correlation: None

SCF Control

Wavefunction Analysis

Frequencies

Raman Frequencies

Isotopic Analysis

Project Out Translational And Rotational Degrees Of Freedom

Compute Anharmonic Corrections

VCI Quanta: 0

Generated Input File:

```

$molecule
0 1
O 0.0000000 0.0184041 -0.0000000
H 0.0000000 -0.5383521 -0.7830360
H -0.0000000 -0.5383521 0.7830360
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Optimization
METHOD = B3LYP
SCF_CONVERGENCE = 8
$end

@@@
|molecule
read
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Frequency
METHOD = B3LYP
SCF_CONVERGENCE = 8
$end

```

Server: QChem

[Reset] [Cancel] [Submit]

← New job starts

← Read the geometry from the previous calculation

- One can manually modify the input preview

- \$rem section

Generated Input File:

```

$molecule
0 1
O 0.0000000 0.0184041 -0.0000000
H 0.0000000 -0.5383521 -0.7830360
H -0.0000000 -0.5383521 0.7830360
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Optimization
METHOD = B3LYP
SCF_CONVERGENCE = 8
$end
  
```

Server: QChem

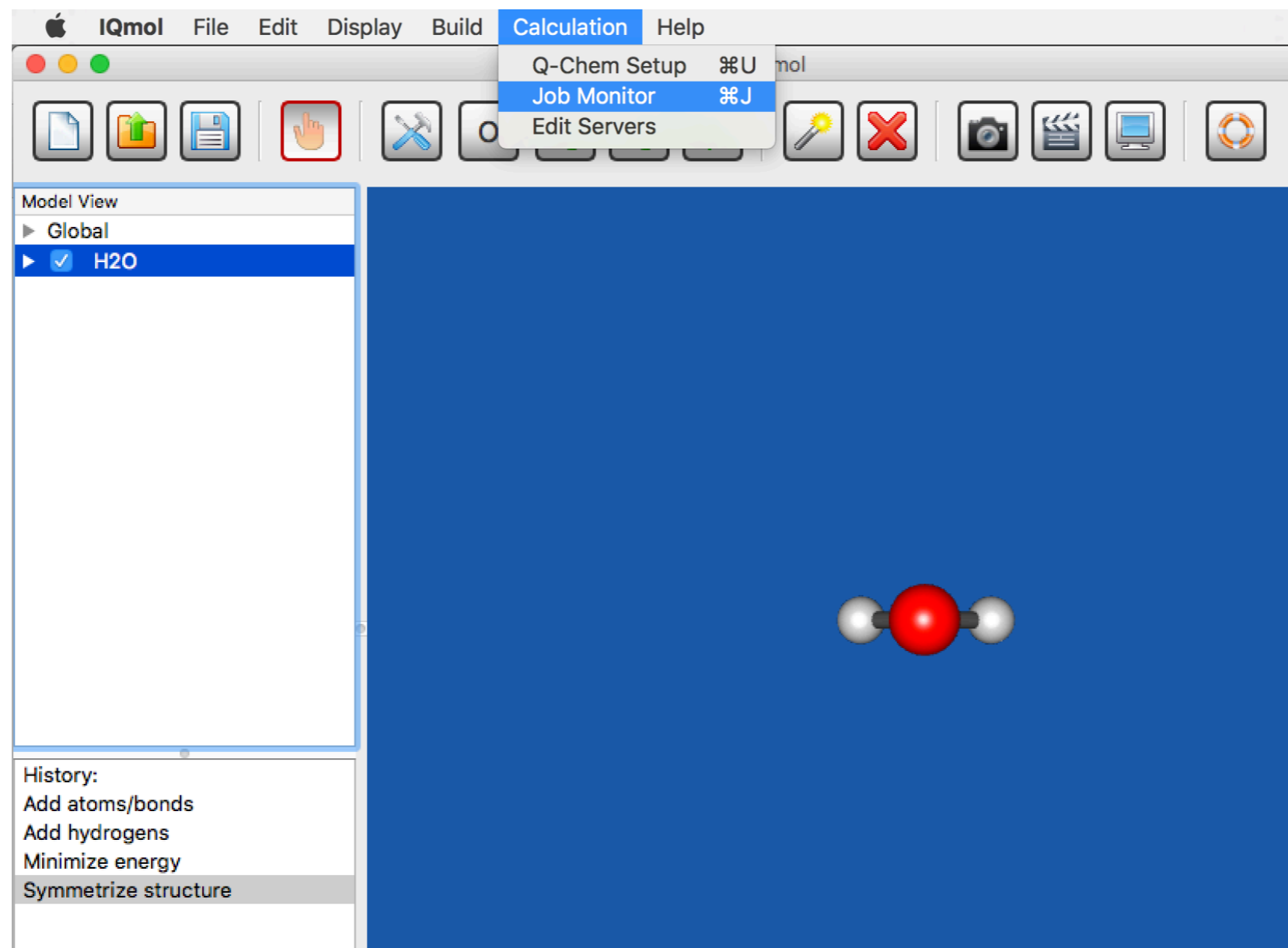
Reset Cancel Submit

- Save the input on a disk: **File** → **save as**
- Use **.inp** for name of the input file

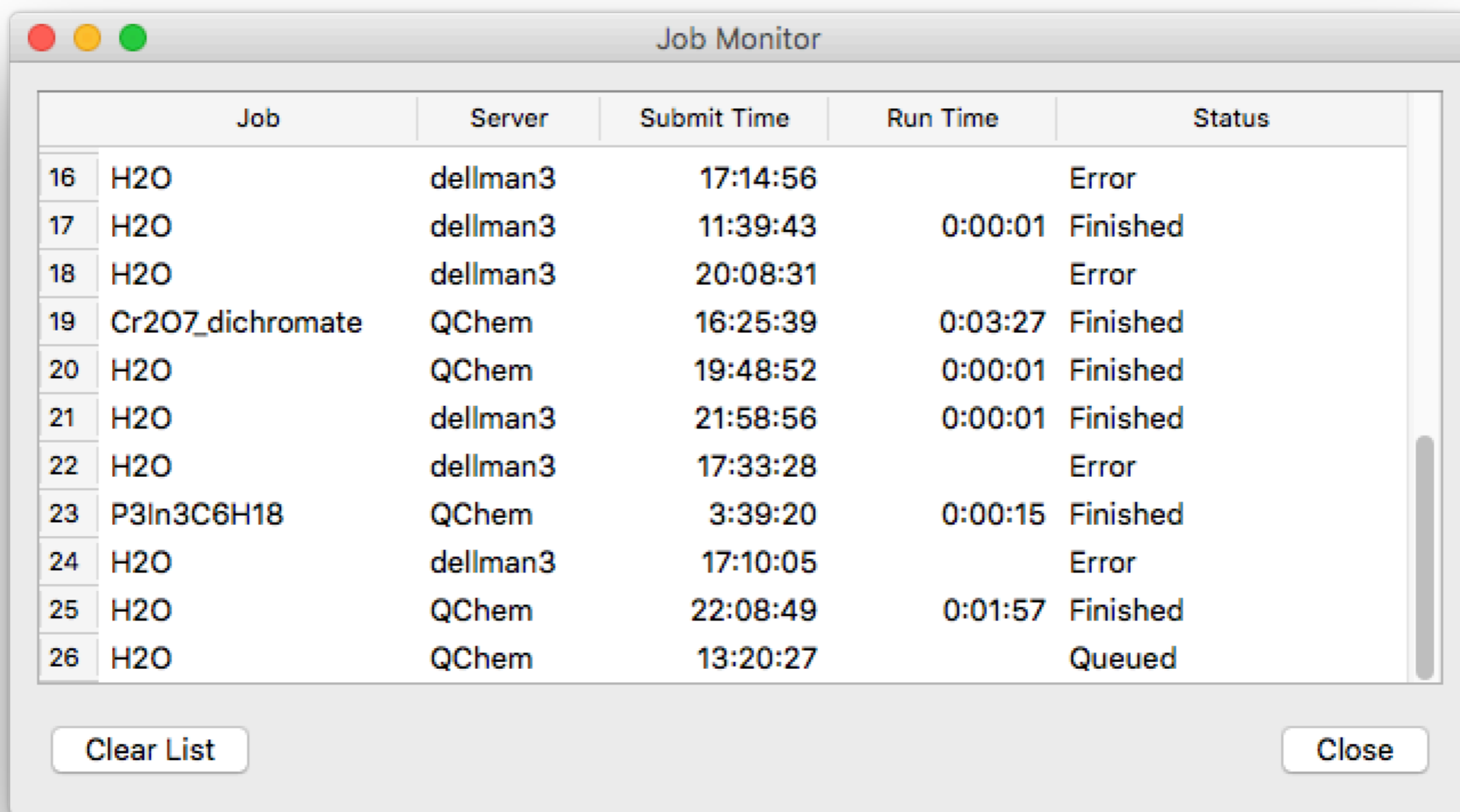
Give a name and remember it.

The screenshot displays the IQmol software interface. On the left, the 'Setup' tab is active, showing configuration options for a job section named 'H2O-opt'. The 'Calculate' dropdown is set to 'Geometry', 'Method' to 'Omega-B97X-V', 'Basis' to '6-31G*', and 'Exchange' to 'HF'. The 'SCF Control' section includes 'Algorithm' set to 'DIIS', 'Guess' to 'SAD', and 'Second Basis' to 'None'. A small dialog box titled 'IQmol' is overlaid on the interface, with the 'Job name:' field containing 'H2O'. On the right, the 'Generated Input File' is shown, containing two input blocks: one for geometry optimization and one for frequency calculation. The server is set to 'QChem'. At the bottom left, the text 'Obtaining job name' is visible.

- Check the job status by selecting: **“Calculation —>Job Monitor”**



- Check the job status by selecting: **“Calculation → Job Monitor”**



The screenshot shows a window titled "Job Monitor" with a table of job details. The table has five columns: Job, Server, Submit Time, Run Time, and Status. The jobs listed are numbered 16 through 26. Jobs 16, 18, 22, and 24 are in an "Error" state, while jobs 17, 19, 20, 21, 23, and 25 are "Finished". Job 26 is "Queued".

	Job	Server	Submit Time	Run Time	Status
16	H2O	dellman3	17:14:56		Error
17	H2O	dellman3	11:39:43	0:00:01	Finished
18	H2O	dellman3	20:08:31		Error
19	Cr2O7_dichromate	QChem	16:25:39	0:03:27	Finished
20	H2O	QChem	19:48:52	0:00:01	Finished
21	H2O	dellman3	21:58:56	0:00:01	Finished
22	H2O	dellman3	17:33:28		Error
23	P3In3C6H18	QChem	3:39:20	0:00:15	Finished
24	H2O	dellman3	17:10:05		Error
25	H2O	QChem	22:08:49	0:01:57	Finished
26	H2O	QChem	13:20:27		Queued

Buttons: Clear List, Close

■ Job status:

use left mouse button to select the job

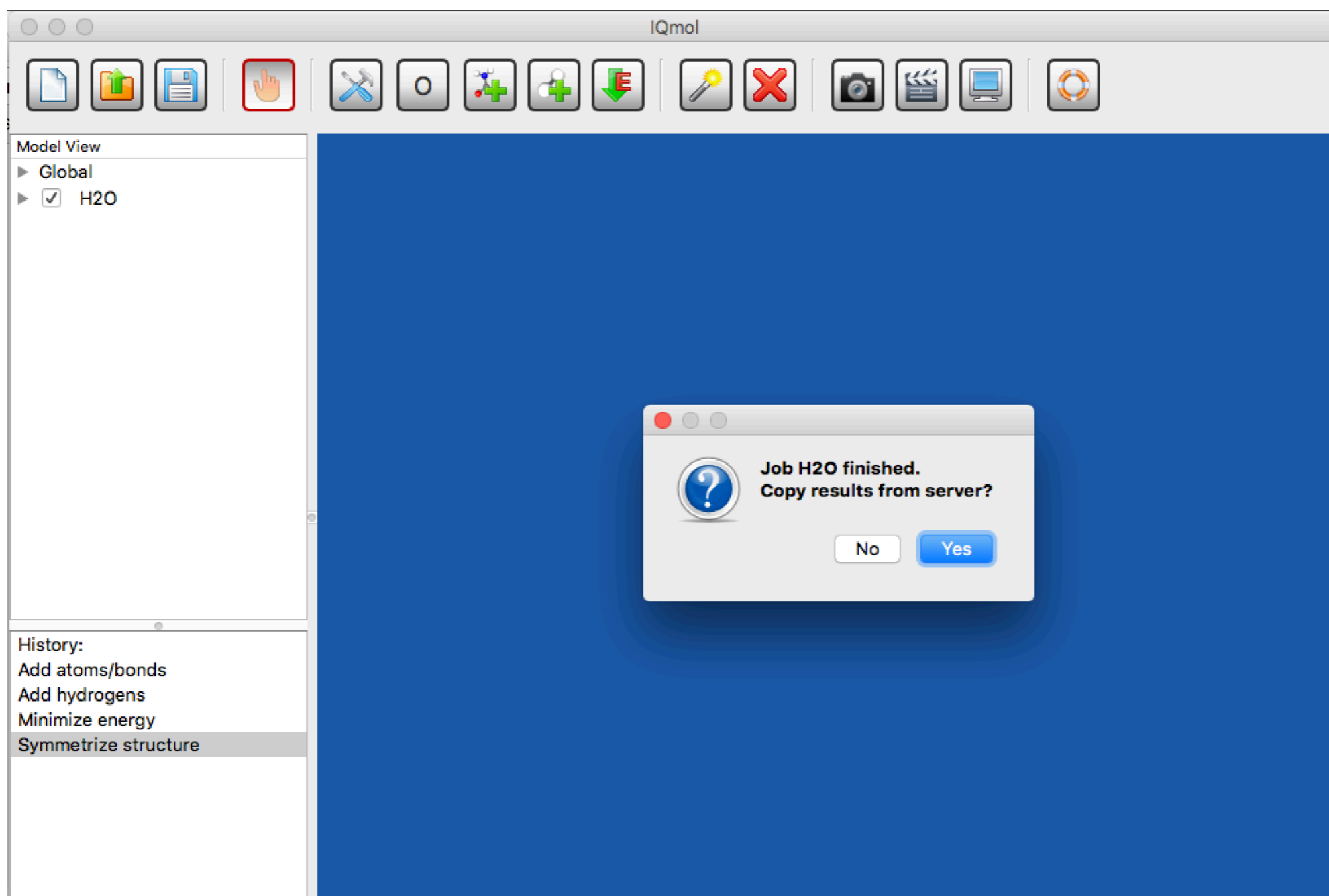
Job	Server	Submit Time	Run Time	Status
16	H2O	dellman3	17:14:56	Error
17	H2O	dellman3	11:39:43	0:00:01 Finished
18	H2O	dellman3	20:08:31	0:00:01 Error
19	Cr2O7_dichromate	QChem	16:25:39	0:03:27 Finished
20	H2O	QChem	09:48:52	0:00:01 Finished
21	H2O	dellman3	21:58:56	0:00:01 Finished
22	H2O	dellman3		Error
23	P3In3C6H18	QChem	3:39:20	0:00:15 Finished
24	H2O	dellman3	17:10:05	Error
25	H2O	QChem	22:08:49	0:01:57 Finished
26	H2O	QChem	13:20:27	0:01:38 Finished

Context menu options for Job 18:

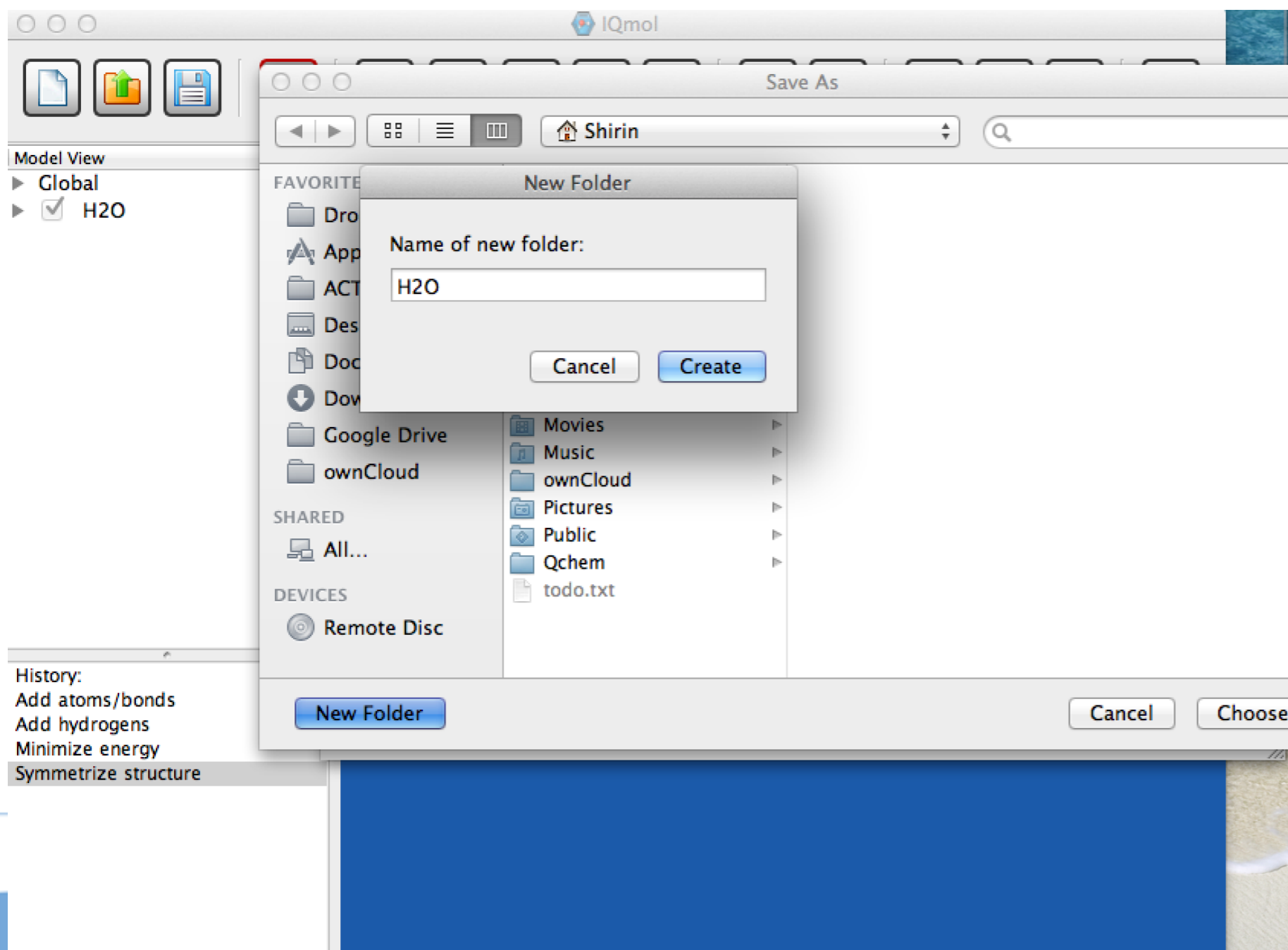
- Kill Job
- Remove Job
- Query Job
- View Output File
- Open Results
- Copy Results From Server

kill the job by selecting this option

use right mouse button to see this menu

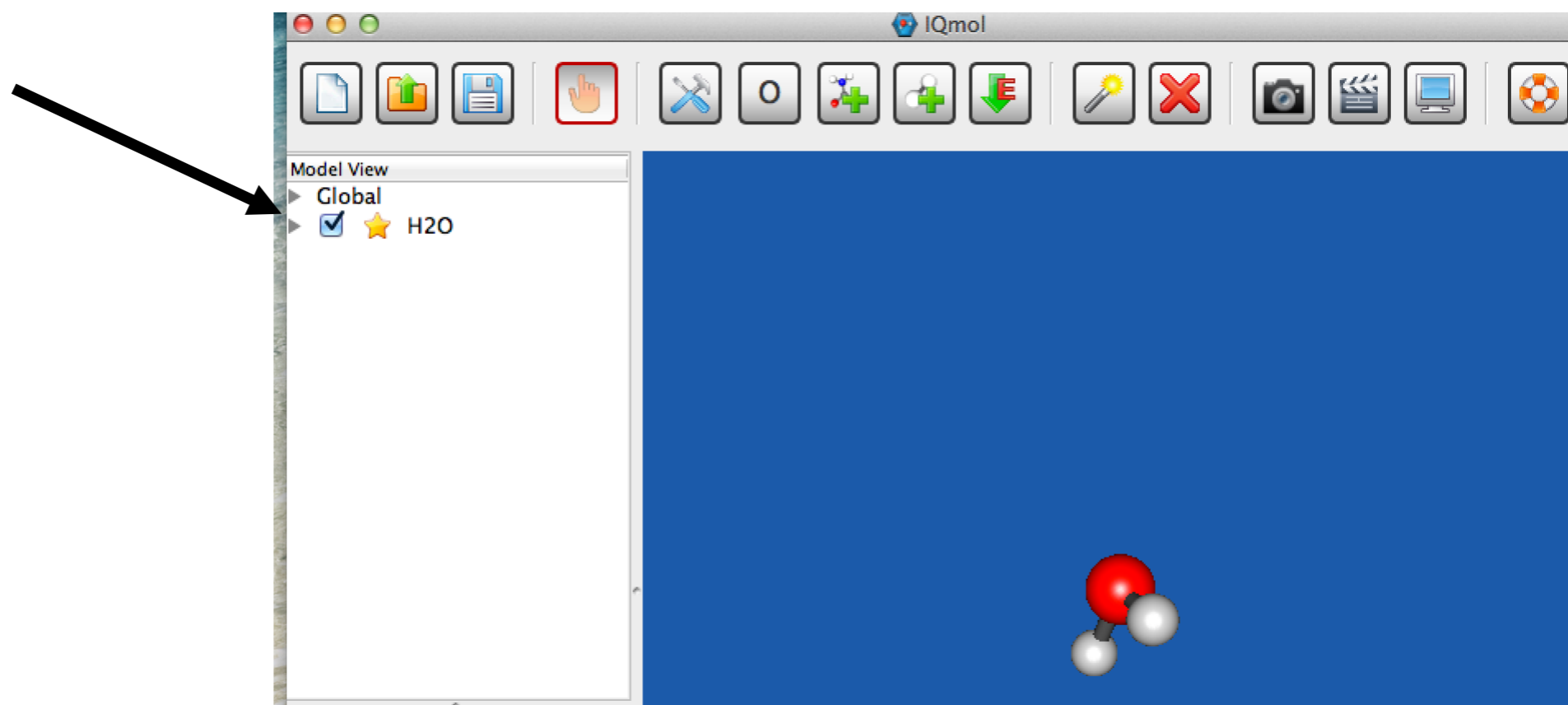


Create new folder to store output files:



Golden star shows that it is copied properly.

Click the checkbox !



- 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

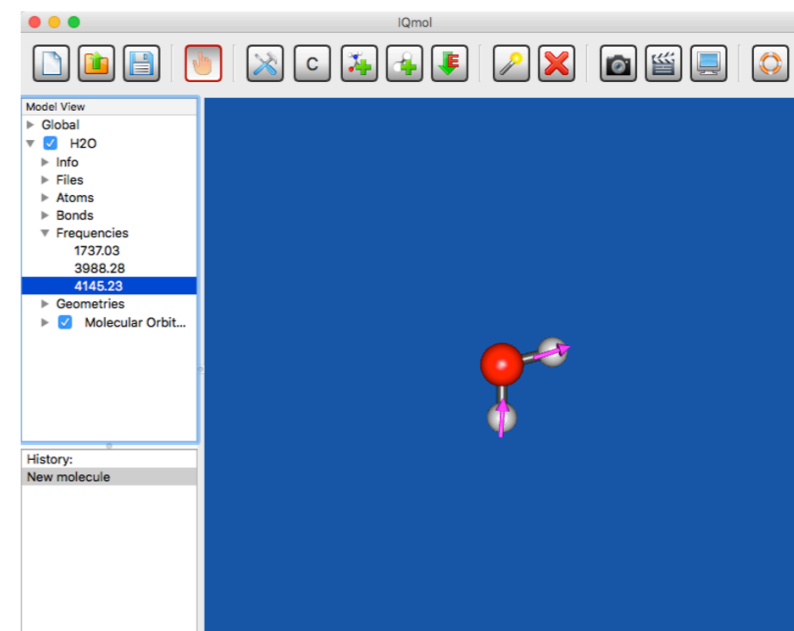
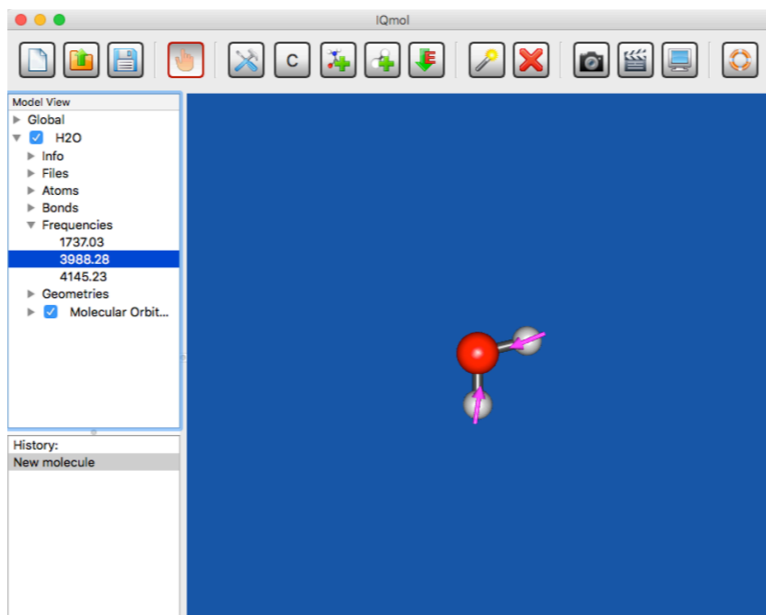
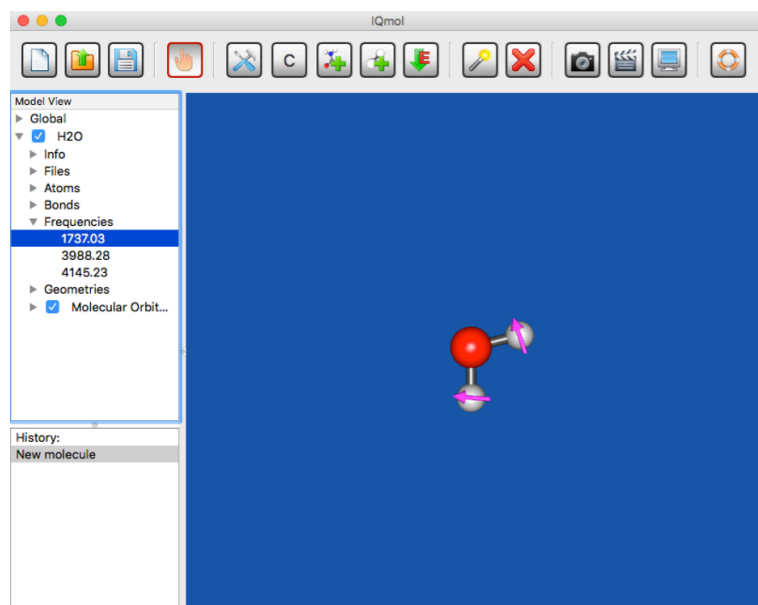
Clicking the arrow next to **Geometries** gives the calculated energy at every step of optimization

The screenshot shows the IQmol software interface. The 'Model View' panel on the left is expanded to show the 'Geometries' section, which contains a list of calculated energies at each step of optimization:

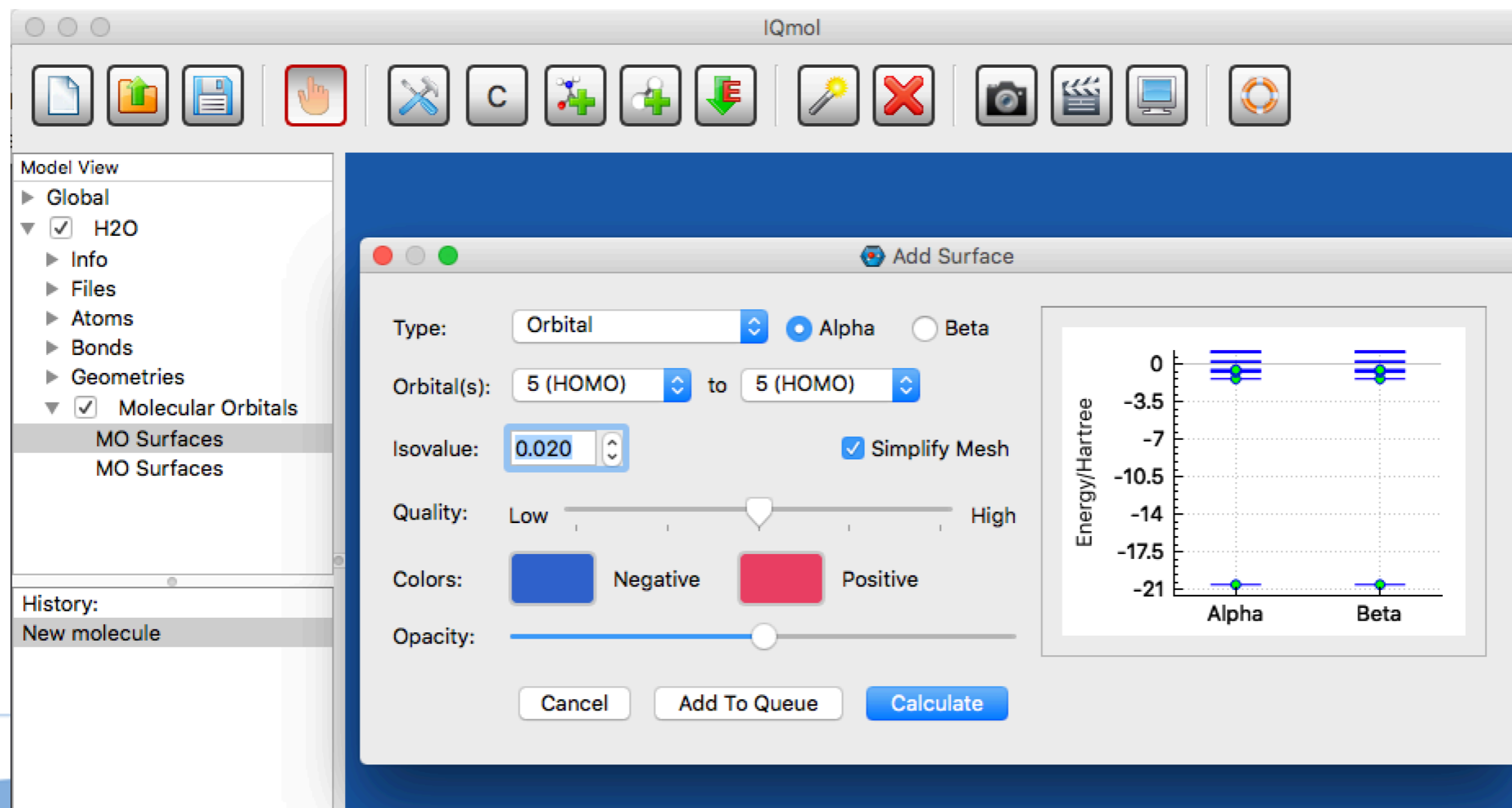
Step	Energy (Hartrees)
1	-75.983457
2	-75.985303
3	-75.985357
4	-75.985359
5	-75.985359

The 'Molecular Orbitals' section is also checked. The main window displays a 3D ball-and-stick model of a water molecule (H₂O) on a blue background.

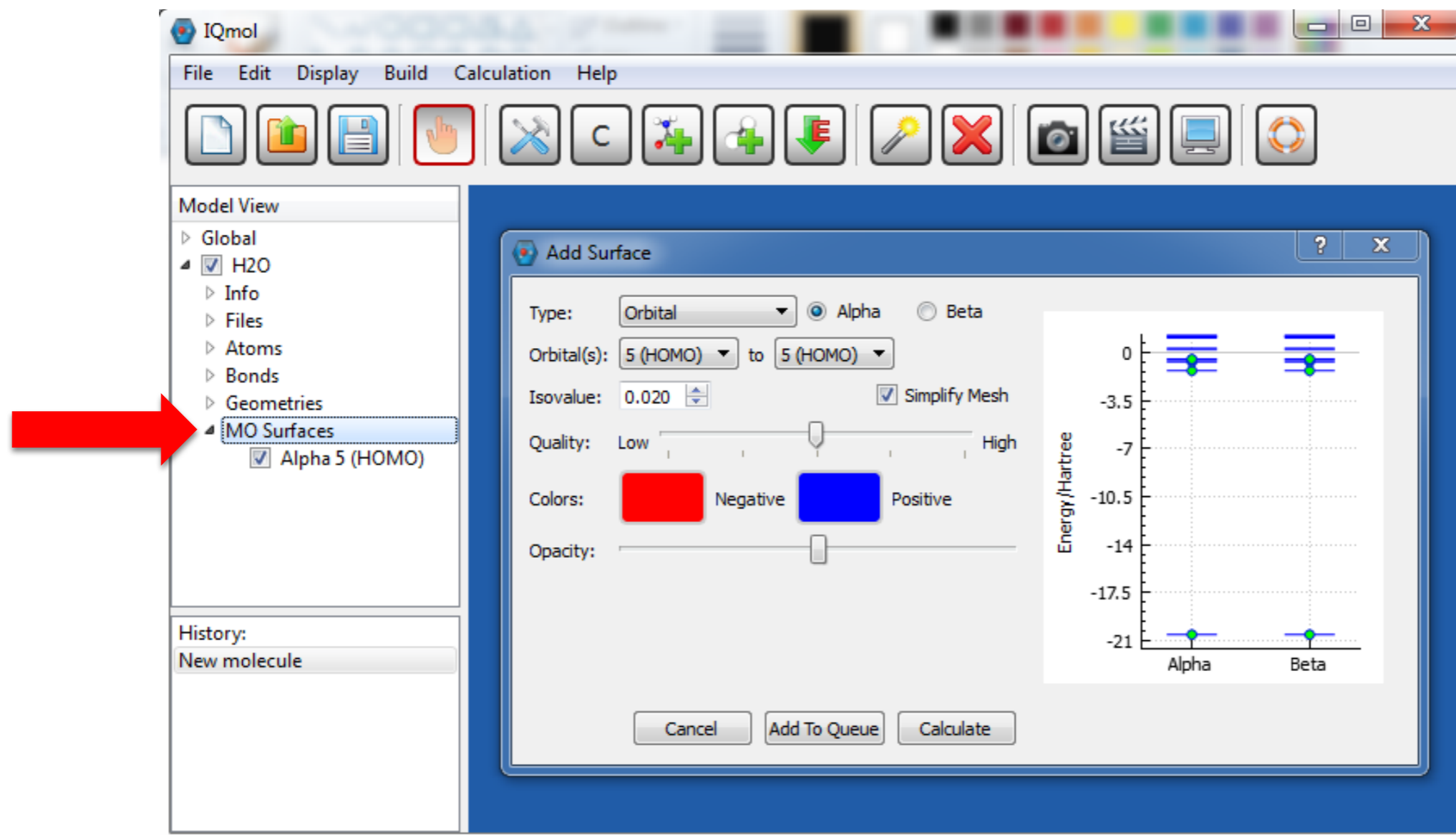
- Clicking the arrow next to **Frequencies** gives the calculated frequencies and displaced vectors for each frequency (for H₂O: 3N-6=3 vibrational frequencies)
- Double click at each value to animate the vibration



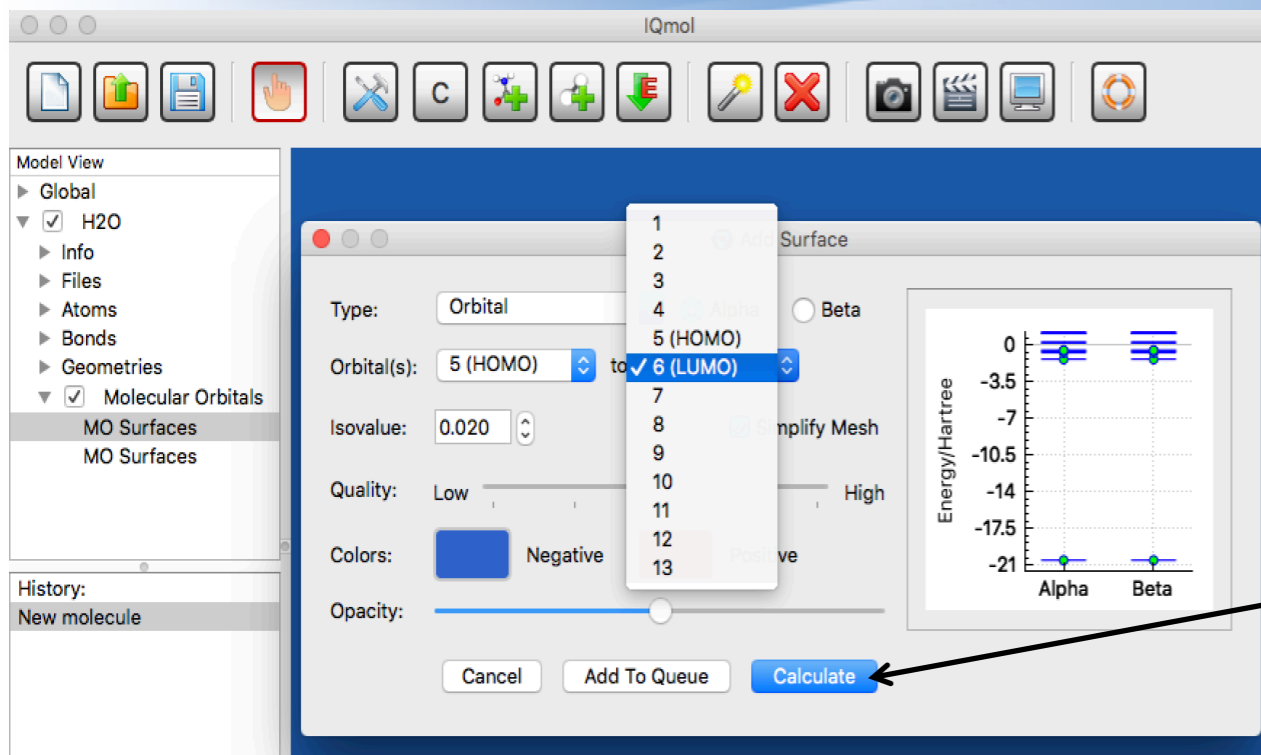
- **Must add GUI = 2 in the \$ rem section** (IQmol does it by default)
- Open **.Fchk** file to see orbitals, density, spin density and so on.
- Double click on **MO Surfaces** under **Molecular Orbitals** (mac) and a window pops up



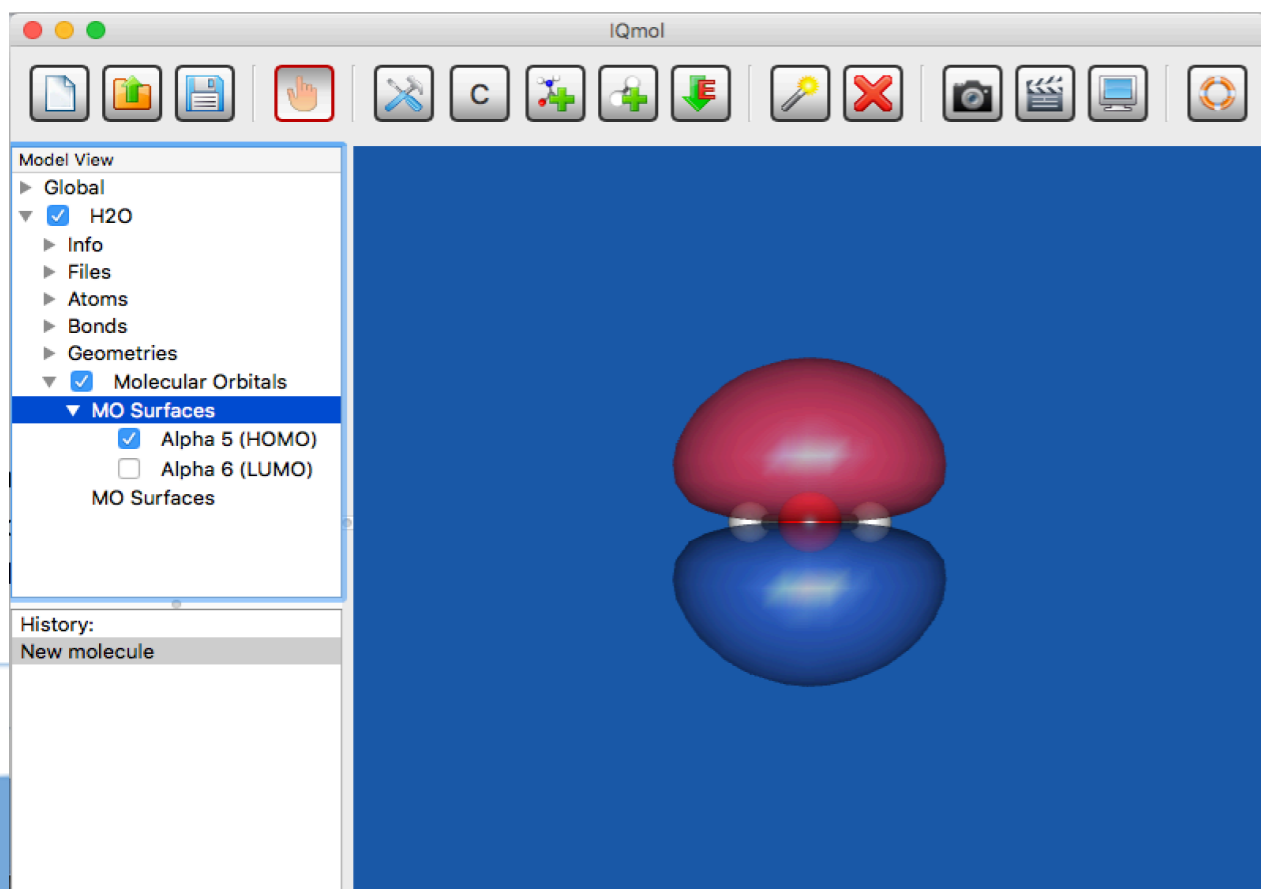
- For **MS Windows** views are little different
- Just double click on **MO Surfaces** and “Add Surface” window pops up



Screen shot from Windows 7

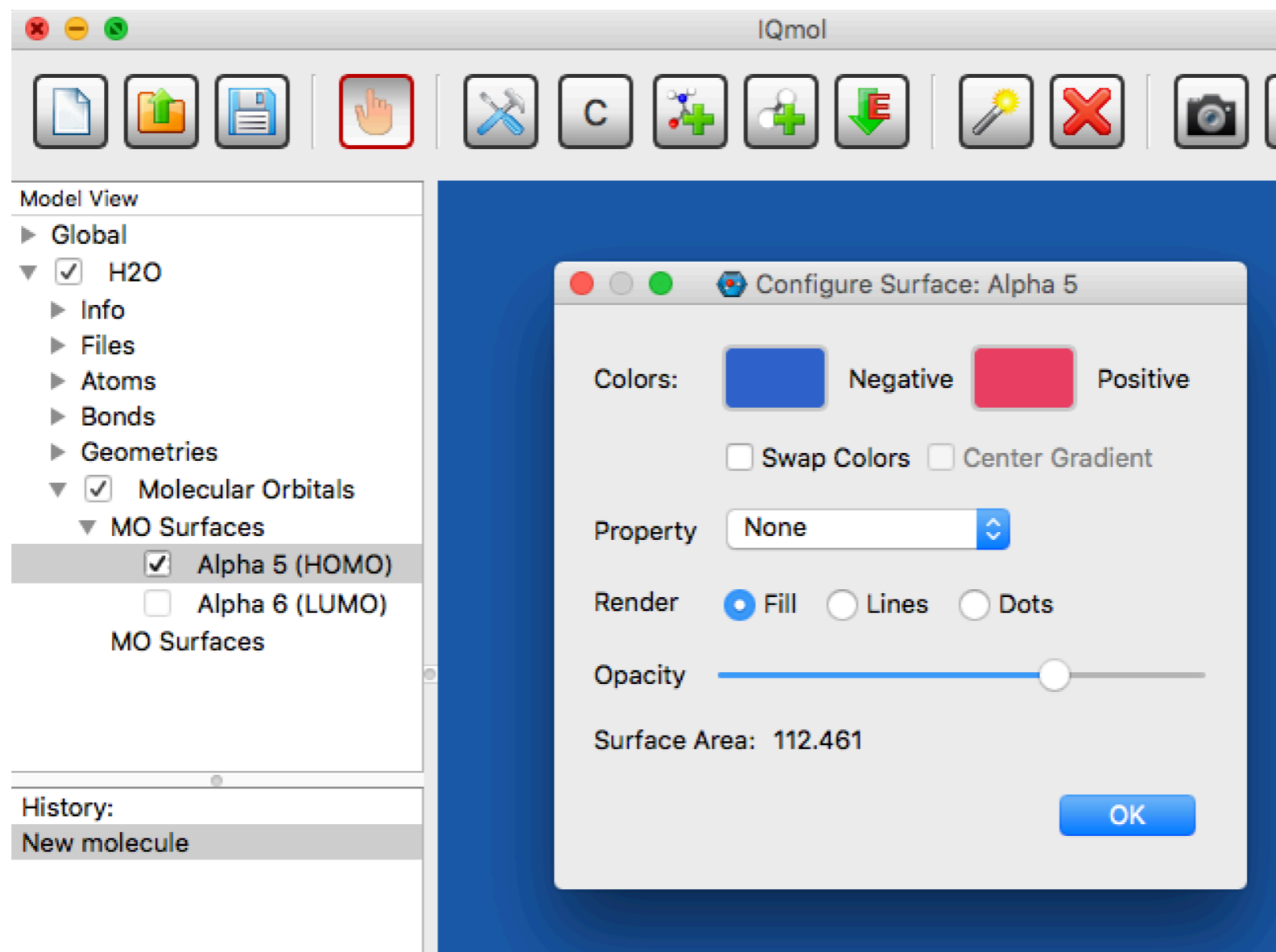


- Select orbital
- Select the relevant orbital (default: HOMO)
- Select the quality you want
- Click **calculate**



- 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.



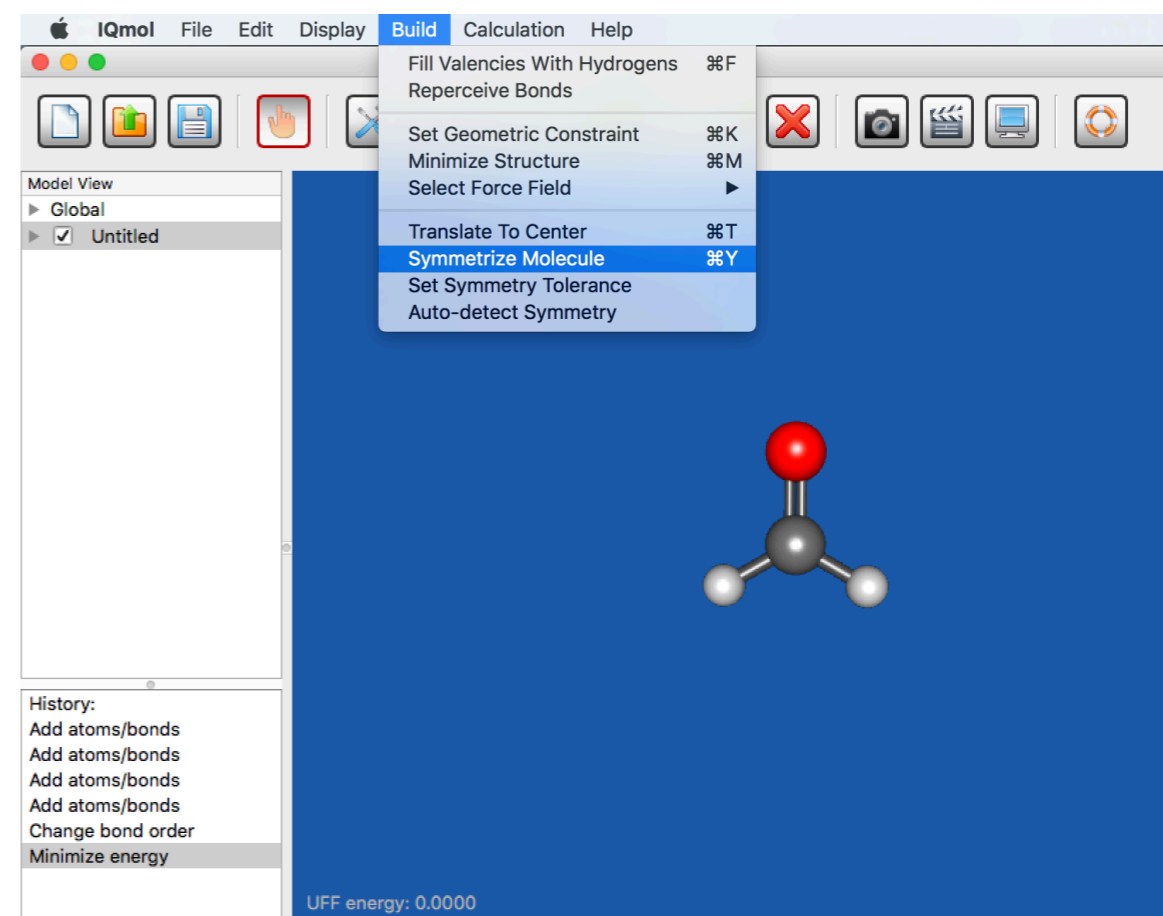
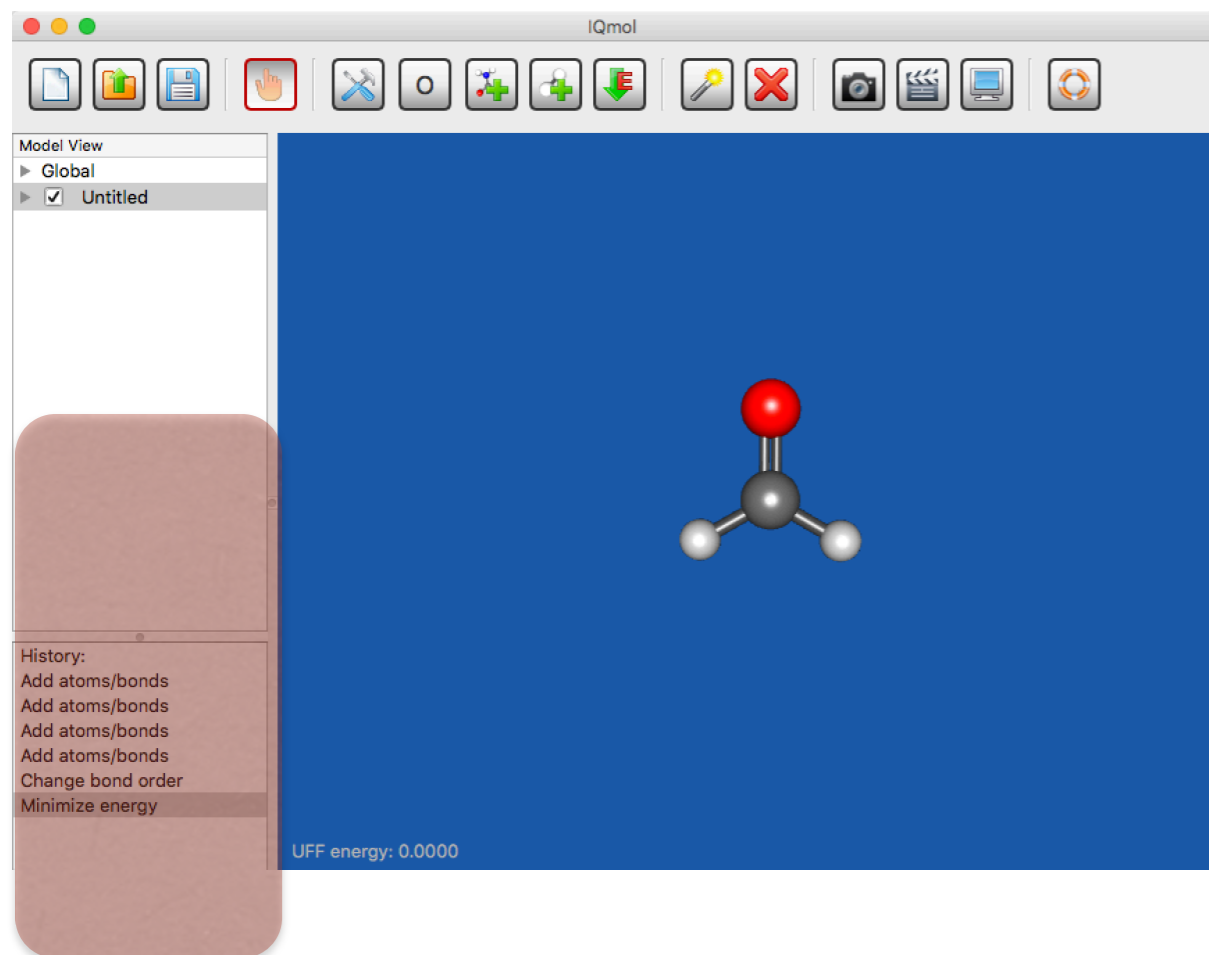
- Double click on **MO Surface** again from MV panel
- “Add Surface” window will pop up again
- Select different properties to be calculated; spin density, density, and so on....

The screenshot displays the IQmol software interface. The main window is titled 'IQmol' and features a toolbar with various icons for file operations, editing, and visualization. On the left, the 'Model View' panel shows a tree structure for the 'H2O' molecule, with 'Molecular Orbitals' and 'MO Surfaces' expanded. Under 'MO Surfaces', 'Alpha 5 (HOMO)' is selected. A 'History' panel at the bottom left shows 'New molecule'. The 'Add Surface' dialog box is open in the foreground, allowing configuration of surface calculations. It includes fields for 'Type' (Density), 'Orbital(s)' (5 (HOMO) to 5 (HOMO)), 'Isovalue' (0.020), 'Quality' (Low to High slider), 'Colors' (Positive, red), and 'Opacity' (slider). A 'Simplify Mesh' checkbox is checked. An energy level diagram on the right shows Energy/Hartree on the y-axis (ranging from -21 to 0) and Alpha/Beta on the x-axis, with orbitals represented by horizontal lines and dots.

Performing Q-Chem calculations

Example 2: CH₂O (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



IQmol

Setup Advanced

Job Section: CH2O-opt [Edit] [Add] [Remove]

Calculate: Geometry [Charge: 0]

Method: Omega-B97X-D [Multiplicity: 1]

Basis: 6-31G* [ECP: None]

Exchange: HF [Correlation: None]

SCF Control

Algorithm: DIIS [Convergence: 8]

Guess: SAD [Max Cycles: 50]

Second Basis: None [Guess Mix: 0%]

Dual Basis Energy Unrestricted

Wavefunction Analysis

Generated Input File:

```

$comment
CH2O-opt
$end

$molecule
0 1
C 0.0000000 -0.0000000 -0.6133812
H 0.0000000 -0.9391510 -1.1555702
H 0.0000000 0.9391510 -1.1555702
O -0.0000000 0.0000000 0.6060735
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Optimization
METHOD = wb97XD
SCF_CONVERGENCE = 8
$end

@@@

$comment
CH2O-Freq
$end

$molecule
read
$end

$rem
  
```

Server: QChem

Reset Cancel Submit

IQmol

Setup Advanced

Job Section: CH2O-Freq [Edit] [Add] [Remove]

Calculate: Frequencies Charge: 0

Method: Omega-B97X-D Multiplicity: 1

Basis: 6-31G* ECP: None

Exchange: HF Correlation: None

SCF Control

Wavefunction Analysis

Frequencies

Raman Frequencies

Isotopic Analysis

Project Out Translational And Rotational Degrees Of Freedom

Compute Anharmonic Corrections

VCI Quanta: 0

Generated Input File:

```

H 0.000000 0.9391510 -1.1555702
O -0.000000 0.000000 0.6060735
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Optimization
METHOD = wB97XD
SCF_CONVERGENCE = 8
$end

@@@

$comment
CH2O-Freq
$end

$molecule
read
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Frequency
METHOD = wB97XD
SCF_CONVERGENCE = 8
$end

```

Server: QChem

Reset Cancel Submit

The screenshot displays the IQmol software interface. The main window is titled "IQmol" and has two tabs: "Setup" and "Advanced". The "Advanced" tab is active, showing various computational chemistry parameters.

Job Section: CH20-opt

Calculate: Geometry

Method: Omega-B97X-D

Basis: 6-31G*

Exchange: HF

Charge: 0

Multiplicity: 1

ECP: None

Correlation: None

SCF Control:

- Algorithm: DIIS
- Guess: SAD
- Second Basis: None
- Dual Basis Energy:
- Unrestricted:

A small dialog box titled "Job name:" is overlaid on the main window, with a text input field containing "CH20" and "OK" and "Cancel" buttons.

Generated Input File:

```

$comment
CH20-opt
$end

$molecule
0 1
C 0.0000000 -0.0000000 -0.6133812
H 0.0000000 -0.9391510 -1.1555702
H 0.0000000 0.9391510 -1.1555702
O -0.0000000 0.0000000 0.6060735
$end

$rem
BASIS = 6-31G*
GUI = 2
JOB_TYPE = Optimization
METHOD = wb97XD
SCF_CONVERGENCE = 8
$end

@@@

$comment
CH20-Freq
$end

$molecule
read
$end

$rem
  
```

At the bottom right of the main window, there is a "Server" dropdown menu set to "QChem", and buttons for "Reset", "Cancel", and "Submit".

At the bottom left of the screenshot, the text "Obtaining job name" is visible.

The screenshot shows the IQmol software interface. The menu bar includes Apple, IQmol, File, Edit, Display, Build, Calculation, and Help. The 'Calculation' menu is open, showing options: Q-Chem Setup (⌘U), Job Monitor (⌘J), and Edit Servers. The 'Job Monitor' option is highlighted. The toolbar contains various icons for file operations and calculations. The 'Model View' panel on the left shows a tree structure with 'Global' and 'CH2O' (checked and starred). The 'History' panel lists actions such as 'Add atoms/bonds', 'Change bond order', 'Minimize energy', and 'Symmetrize structure'. The main 3D view displays a ball-and-stick model of a formaldehyde molecule (CH₂O), with a red oxygen atom at the top, a grey carbon atom in the center, and two white hydrogen atoms at the bottom.

Job Monitor

	Job	Server	Submit Time	Run Time	Status
31	Cr2O7_dichromate	QChem	16:25:39	0:03:27	Finished
32	H2O	QChem	22:08:49	0:01:57	Finished
33	CH2O	QChem	11:20:08	0:00:20	Finished
34	CH2O	QChem	11:23:59		Finished
35	CH2O	QChem	11:25:04		Finished
36	CH2O	QChem	11:26:25		Finished
37	CH2O	QChem	11:26:56		Finished
38	CH2O	QChem	11:28:03		Queued

The screenshot displays the IQmol software interface. At the top, a toolbar contains various icons for file operations, editing, and simulation. On the left, a 'Model View' panel shows a tree structure with 'Global' and 'CH2O' (checked and starred). Below it, a 'History' panel lists actions such as 'Add atoms/bonds', 'Change bond order', 'Minimize energy', and 'Symmetrize structure'. The main window features a blue background with a 3D ball-and-stick model of a formaldehyde molecule (CH₂O) centered. A dialog box with a question mark icon is overlaid on the model, containing the text 'Job CH2O finished. Copy results from server?' and two buttons: 'No' and 'Yes'.

Copy files to your laptop

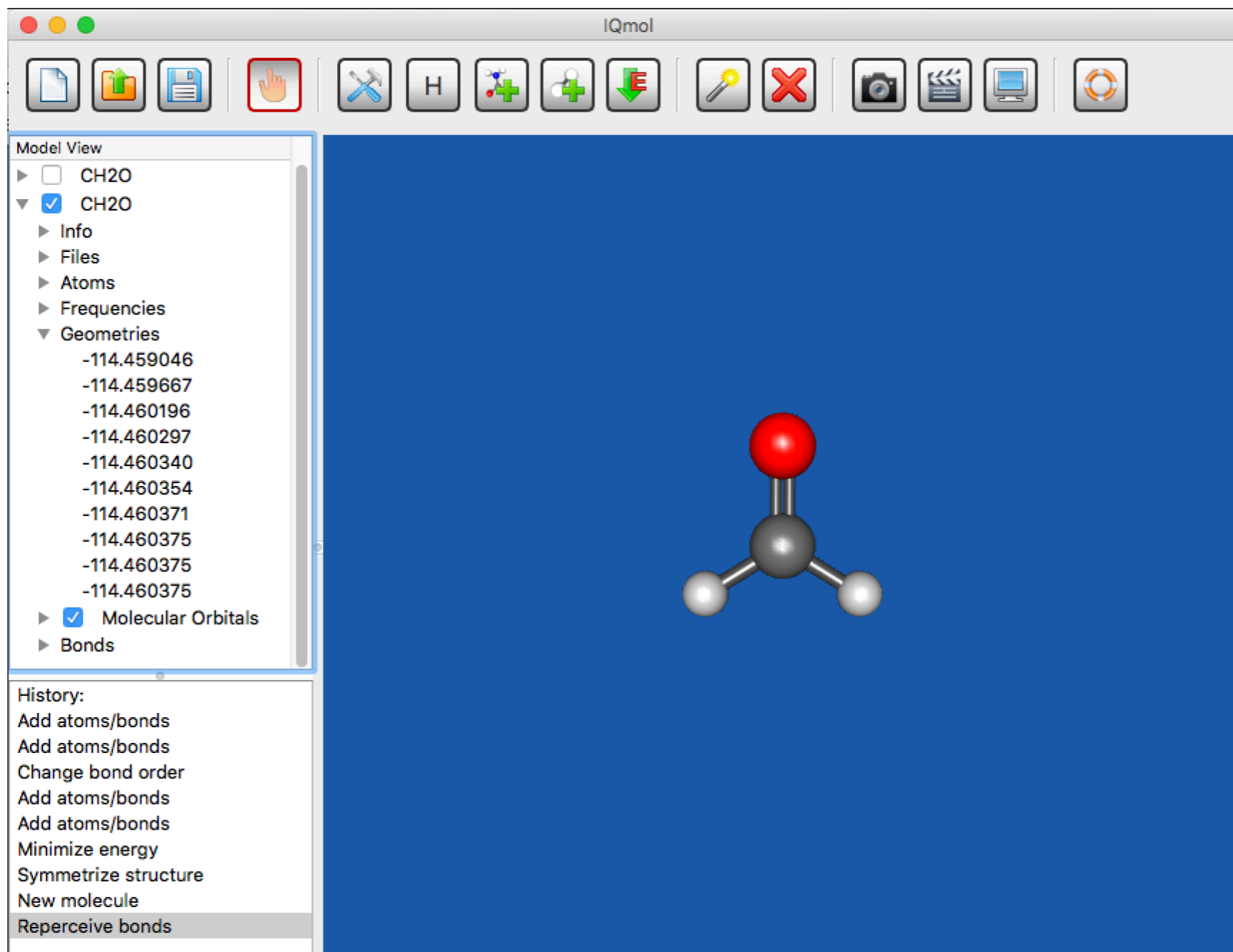
Job Monitor

	Job	Server	Submit Time	Run Time	Status
31	Cr2O7_dichromate	QChem	16:25:39	0:03:27	Finished
32	H2O	QChem	22:08:49	0:01:57	Finished
33	CH2O	QChem	11:20:08	0:00:20	Finished
34	CH2O	QChem	11:23:59		Finished
35	CH2O	QChem	11:25:04		Finished
36	CH2O	QChem	11:26:25		Finished
37	CH2O	QChem	11:26:56		Finished
38	CH2O	QChem	11:28:03	0:00:08	Finished

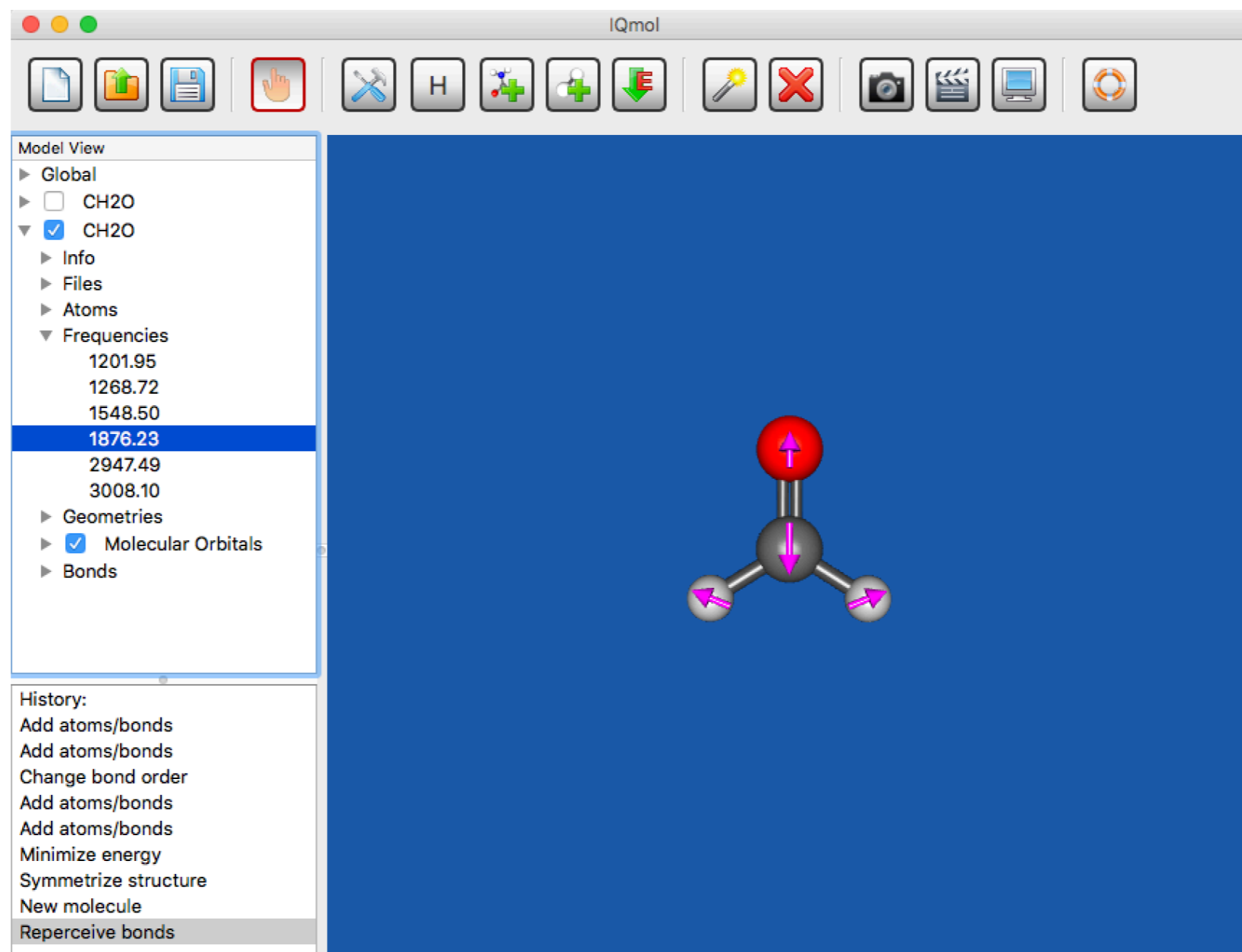
click checkbox



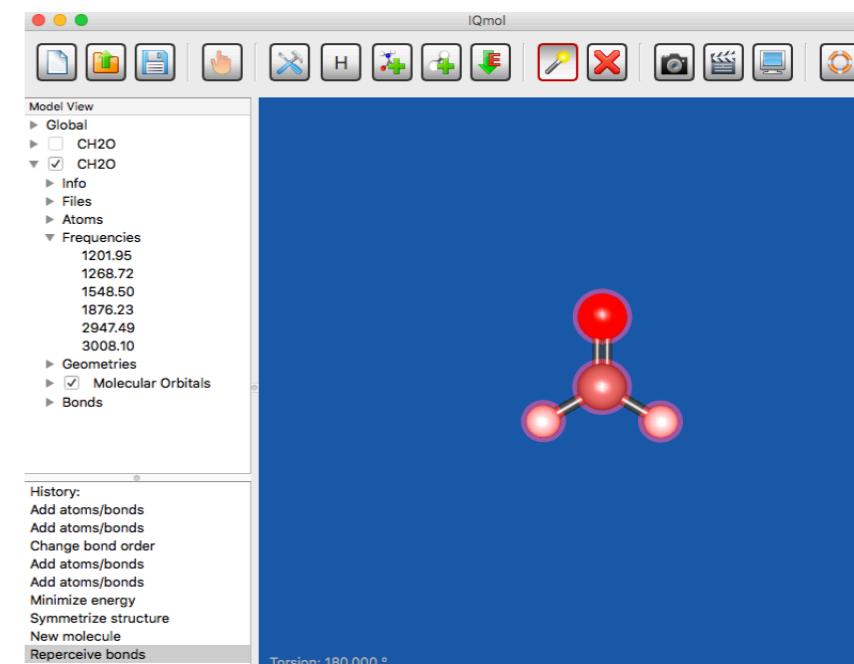
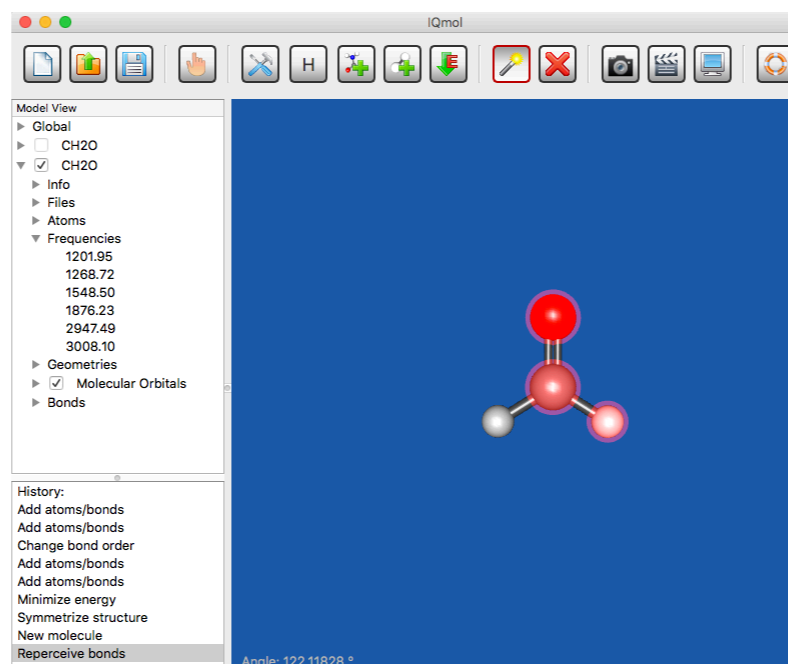
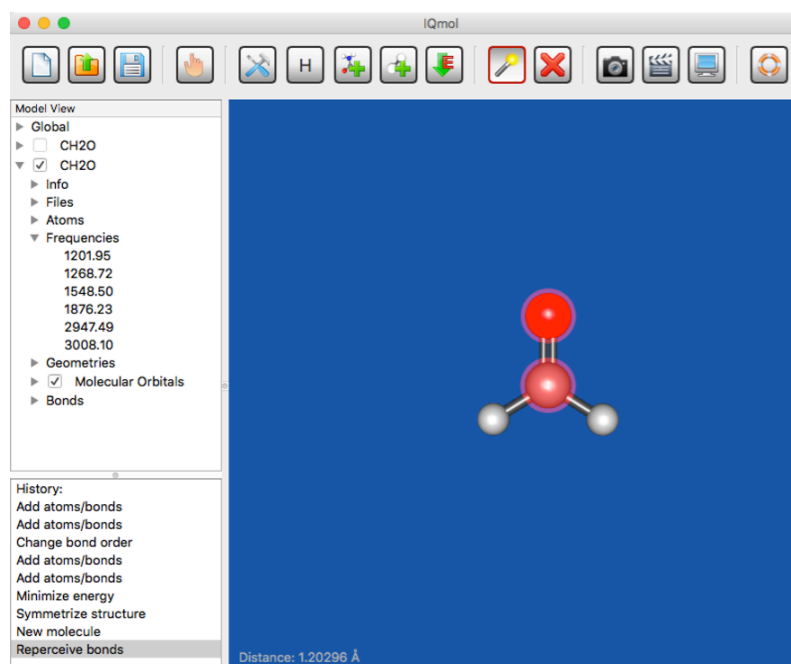
The screenshot shows the IQmol software window. The title bar reads 'IQmol'. The top toolbar contains various icons for file operations, editing, and visualization. On the left, the 'Model View' sidebar is expanded to show the 'CH2O' molecule selected. Underneath, several sub-panels are listed: 'Info', 'Files', 'Atoms', 'Bonds', 'Frequencies', 'Geometries', and 'Molecular Orbitals'. The 'Molecular Orbitals' checkbox is checked. Below the sidebar is a 'History' list with actions like 'Add atoms/bonds', 'Change bond order', 'Minimize energy', and 'Symmetrize structure'. The main window displays a ball-and-stick model of a formaldehyde molecule (CH₂O) with a red oxygen atom, a grey carbon atom, and two white hydrogen atoms.



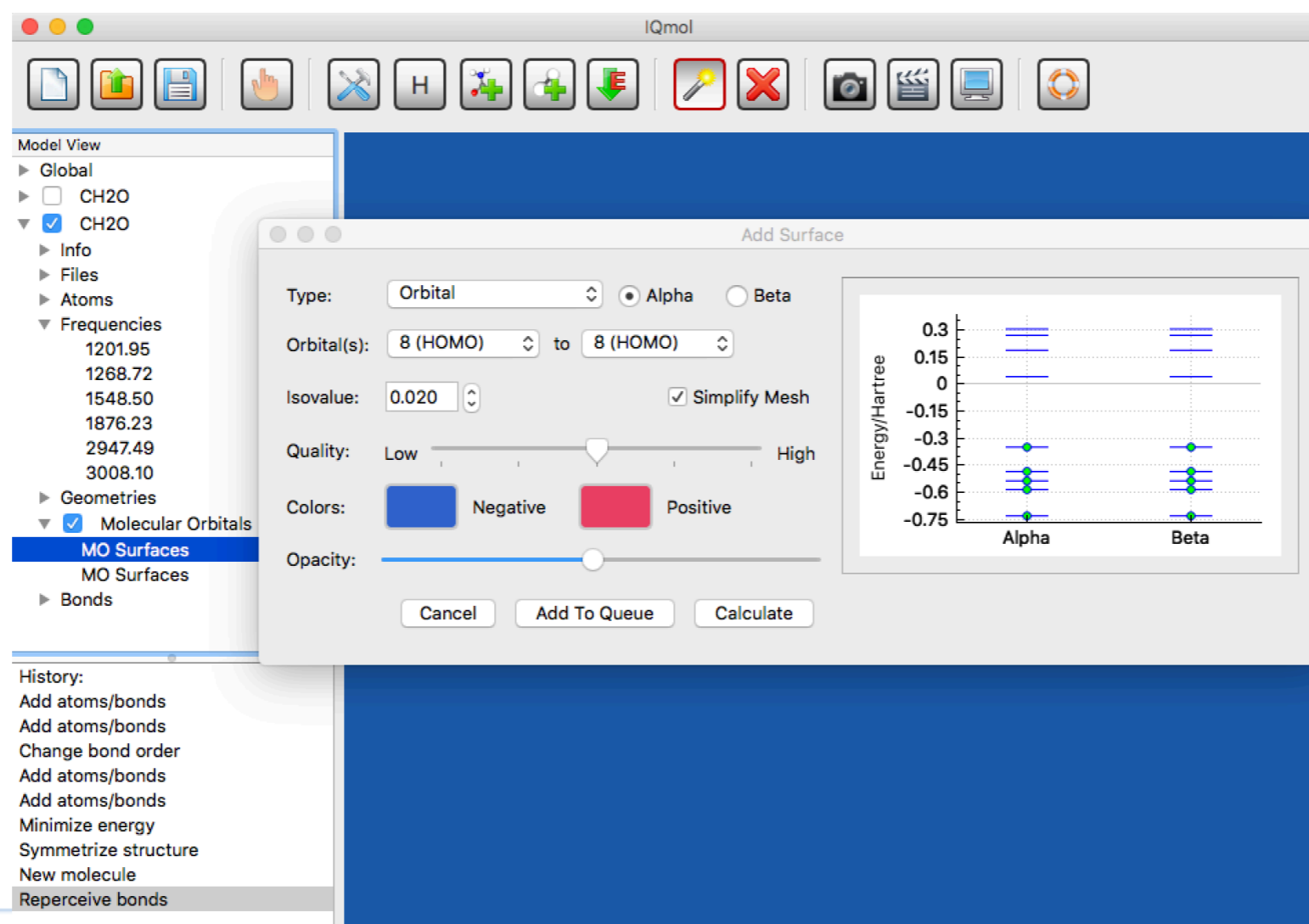
$3N-6=6$ vibrational frequency



- 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 **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**

