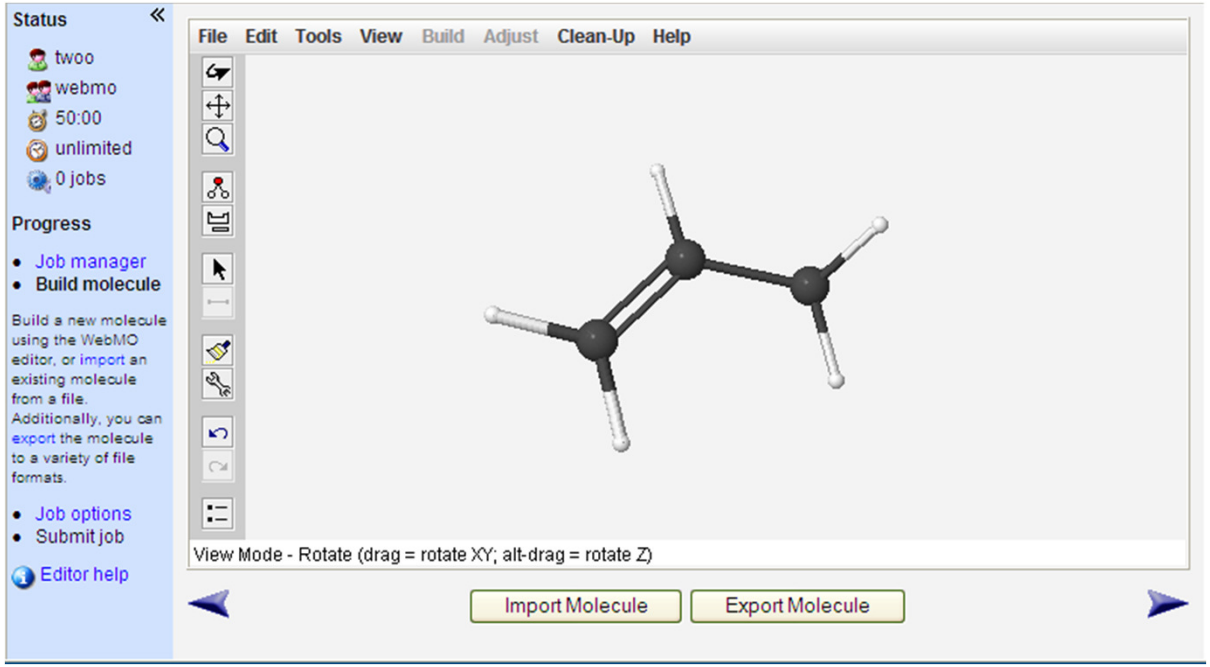
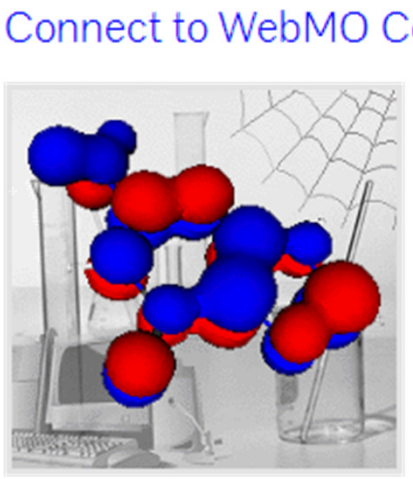
Introduction to WEBMO



- WebMO is a web based graphical user interface to popular quantum chemistry packages like Gaussian.

- You can access it through the course website or directly at:
  http://titan.chem.uottawa.ca/webmo/cgi-bin/login.cgi



WebMO – How it Works

the internet

Java Enabled Web browser on your PC or MAC

- The model builder and interface is run on your web browser.
- Calculations are then submitted to a remote workstation

Woo lab webserver on campus

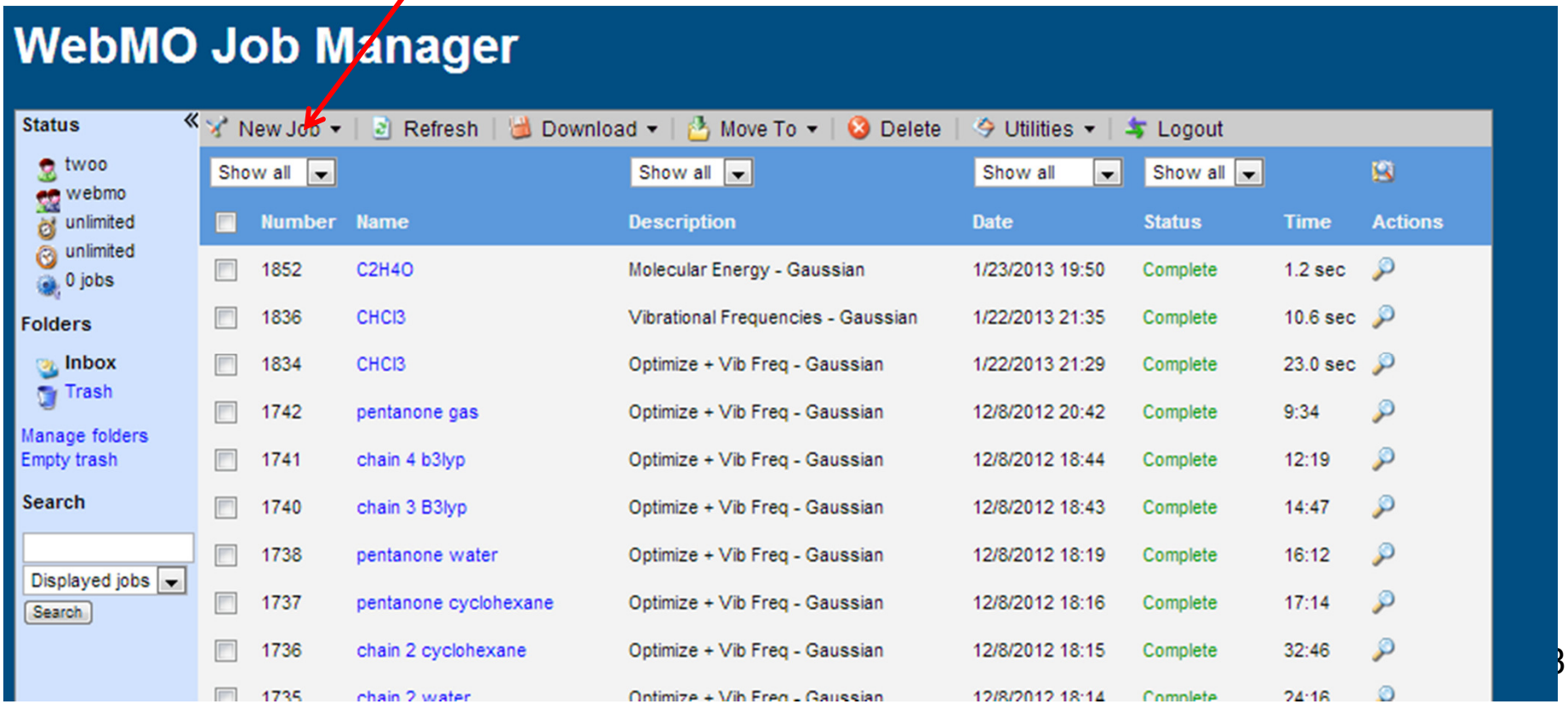
12 CPU core high-end work station

runs Linux

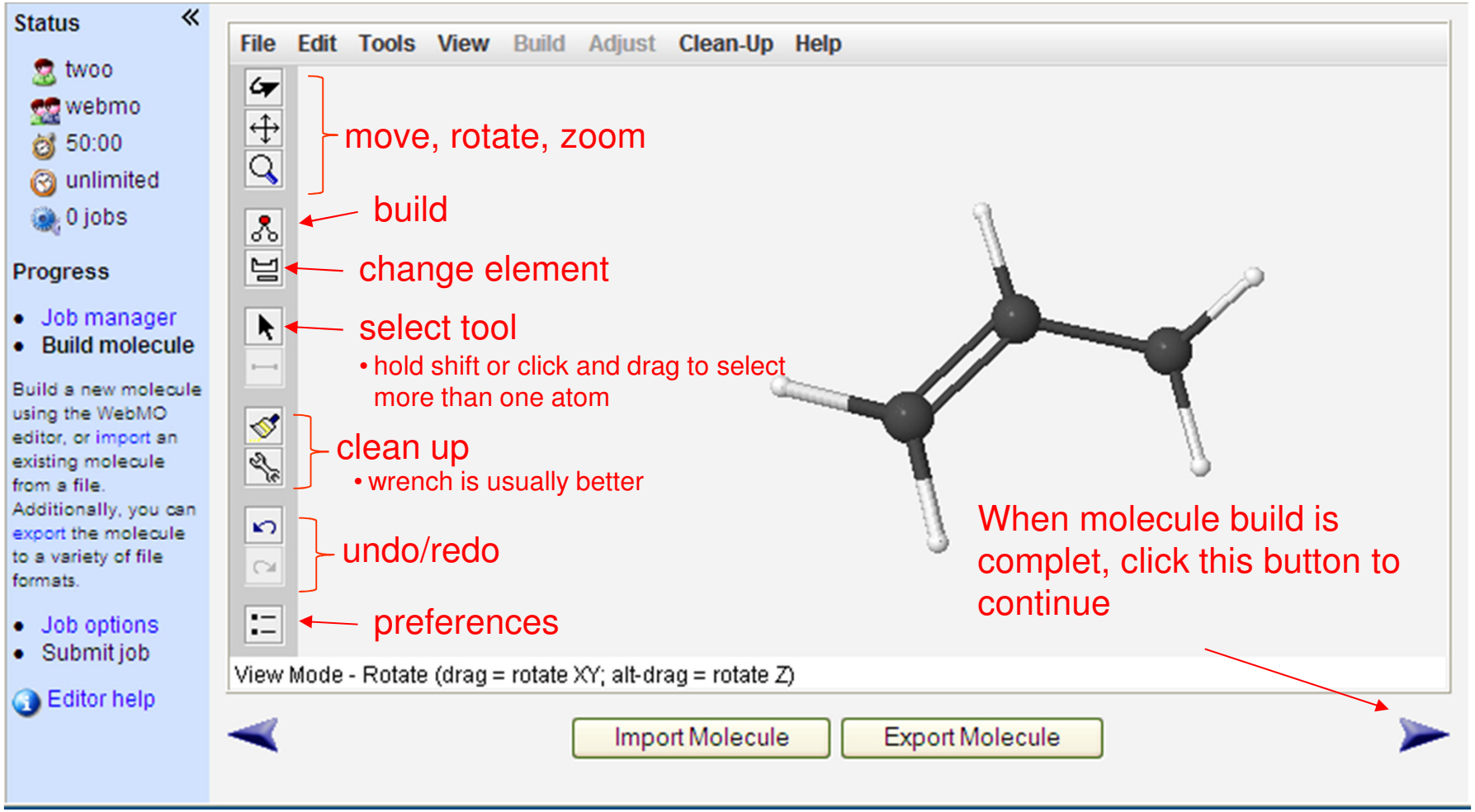
Guassian '09 quantum chemistry package run on server

WebMO – Job Manager

- when you first login, you will be taken to the WebMO Job manager like shown below.
- if you have never logged in before, you will have no jobs and the table below will be empty. (We will revisit the job manager in a later slide)
- click on the 'New Job' button



Web MO – Build Molecule Window

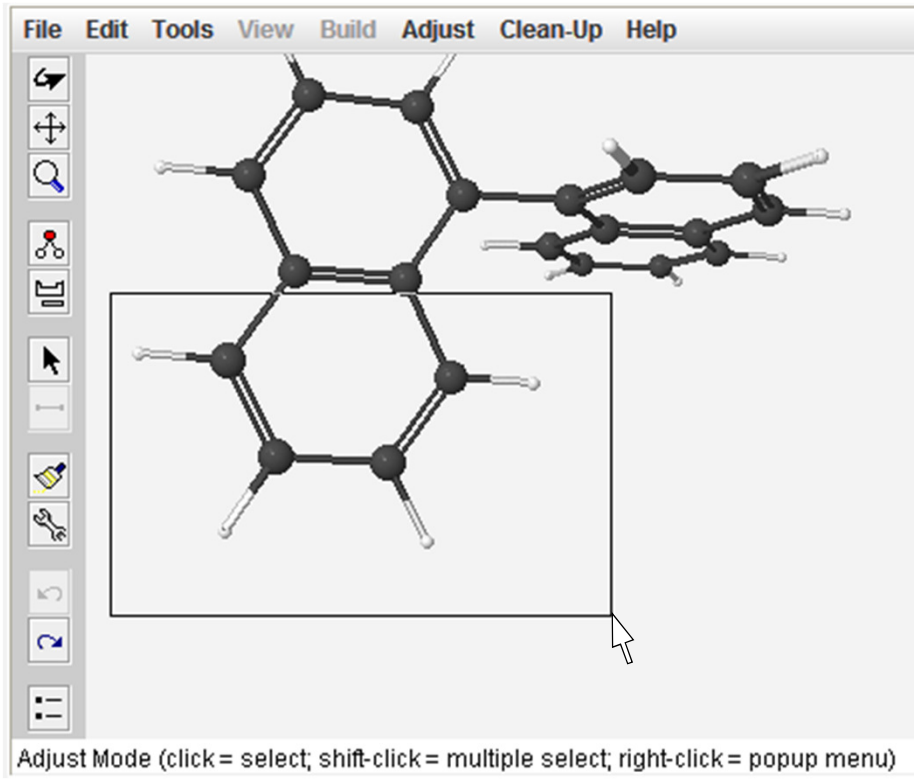


Web MO – Molecule Building

To change an atom's type (element) click on the periodic table icon.

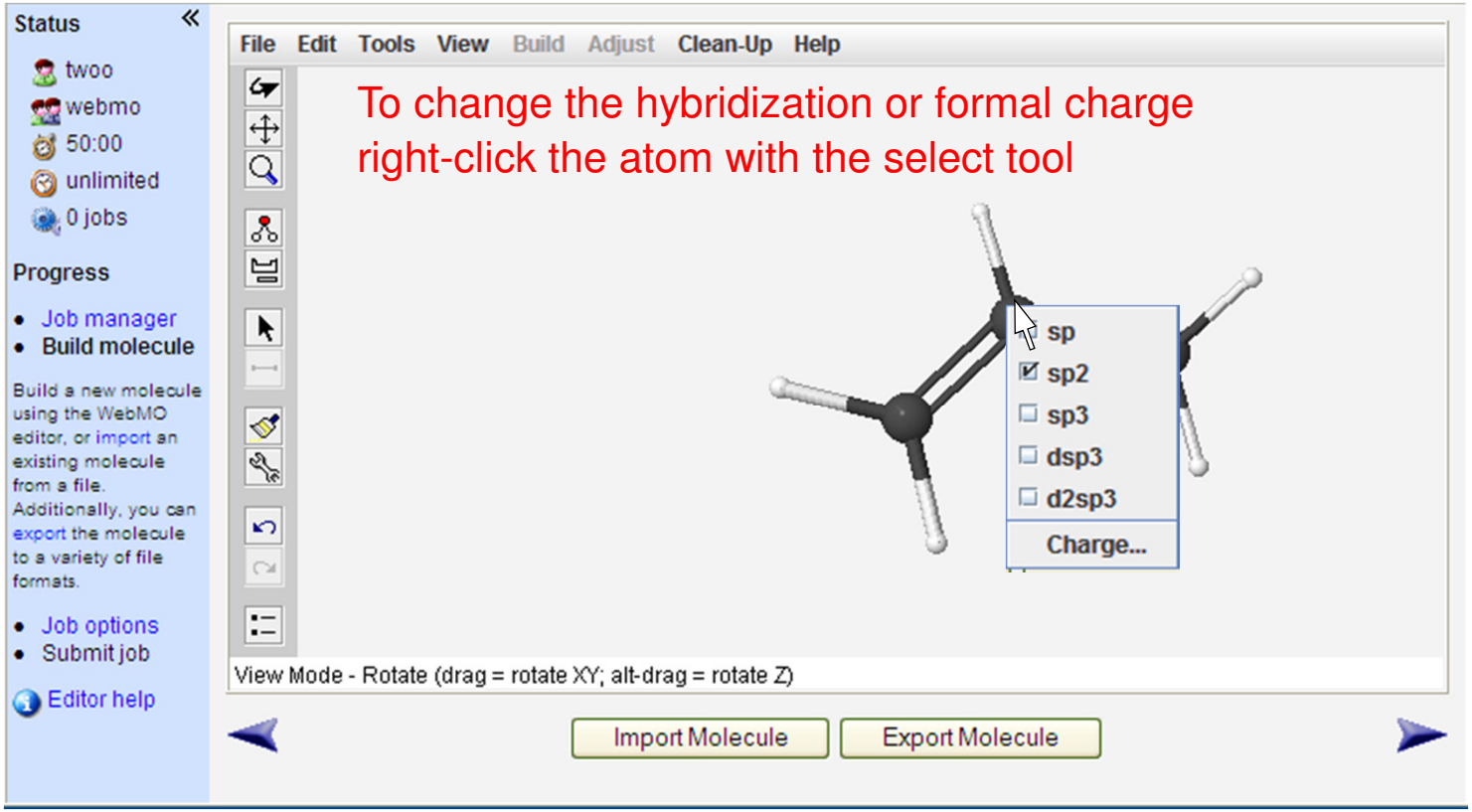
Then click on the atom that you want to change.

To **delete** an atom, select the atoms you want to delete

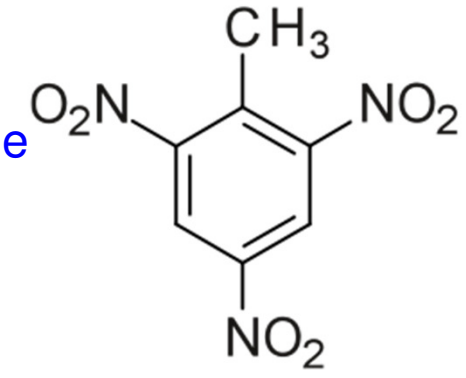


Then use the 'backspace' or 'del' keys on the keyboard

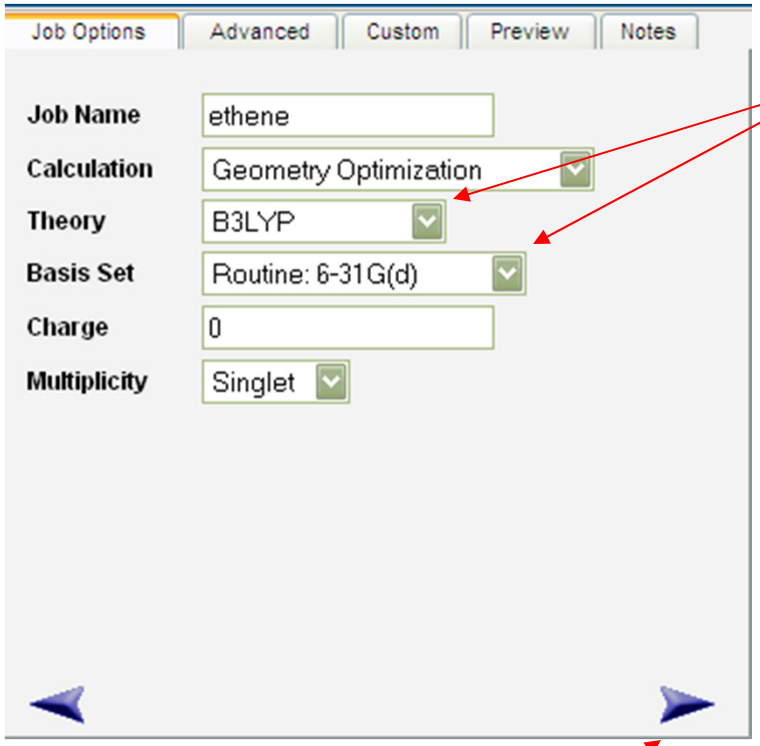
Web MO – Molecule Building



Example: The TNT molecule



Web MO – Configure Job Window



Click on this button to submit the job.

- We will learn about the mean of all of these during the course
- Many of the options are intuitive (explore but…)
- WebMO is an interfaces to G09 and other quantum chemistry packages.
- WebMO simply creates a G09 input (as shown below) and submits the job for you.
- Clicking on the 'Preview' tab gives the raw input:

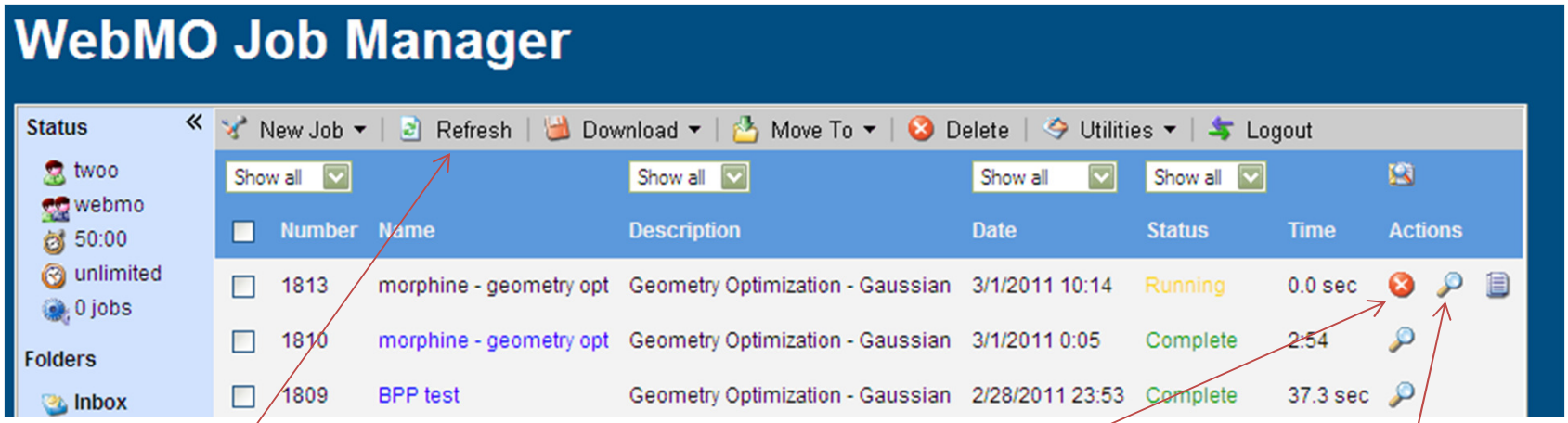
  the raw Gaussian input as shown below can then be edited

```
#N B3LYP/6-31G(d) OPT(EstmFC)

morphine - geometry opt

0 1
C 0.00000000 0.00000000 0.00000000
C 0.69569700 -1.26206200 -0.41503400
C 0.17399600 -2.28866100 -1.18008600
C 1.02208100 -3.36536800 -1.47276900
C 2.35569400 -3.35396600 -1.07771900
C 2.91470000 -2.23285600 -0.43245700
C 2.05974300 -1.17008200 -0.12607500
```

Web MO – Job Manager revisited

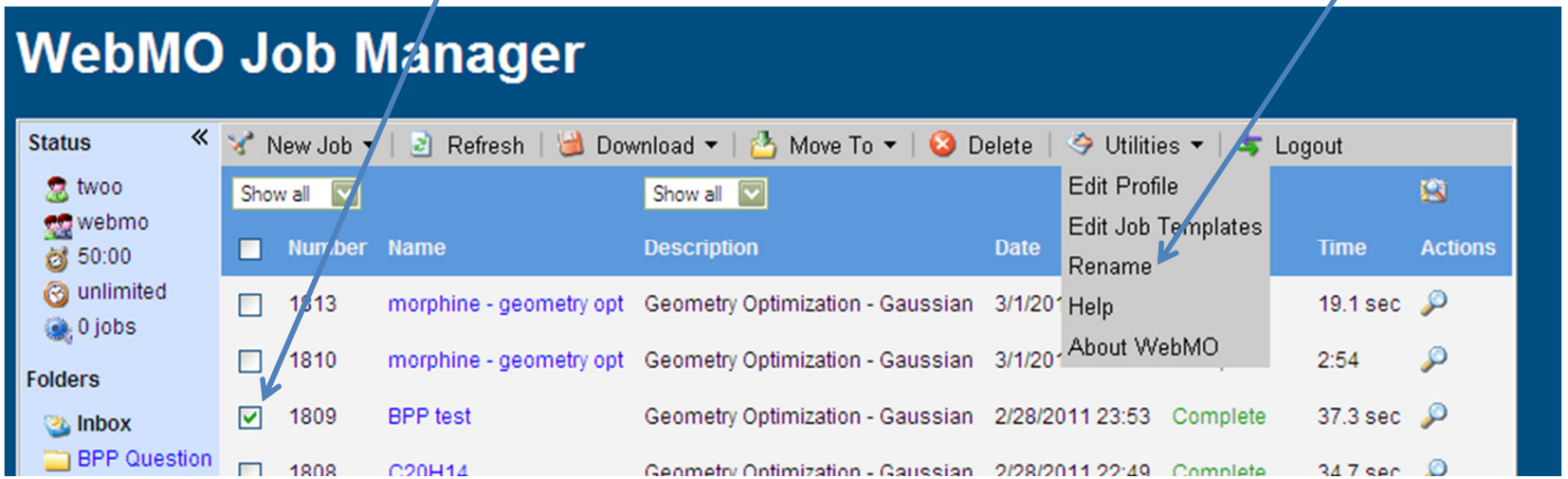


Update the list

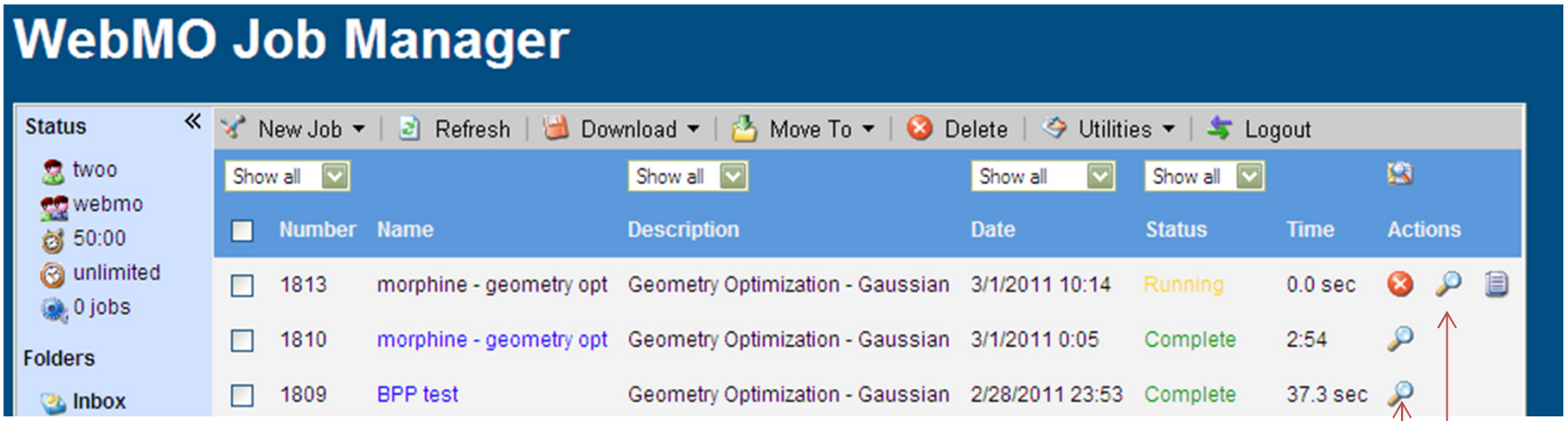
Kill or stop an active job

View progress of job

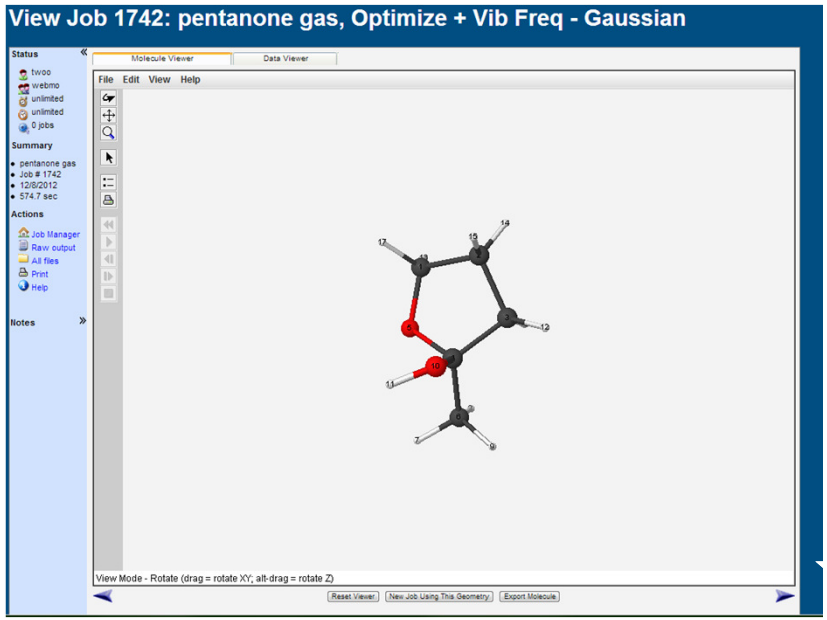
To **rename** a job, select the job, then in the 'Utilities' menu click 'Rename'



How to View the Results of a Job?



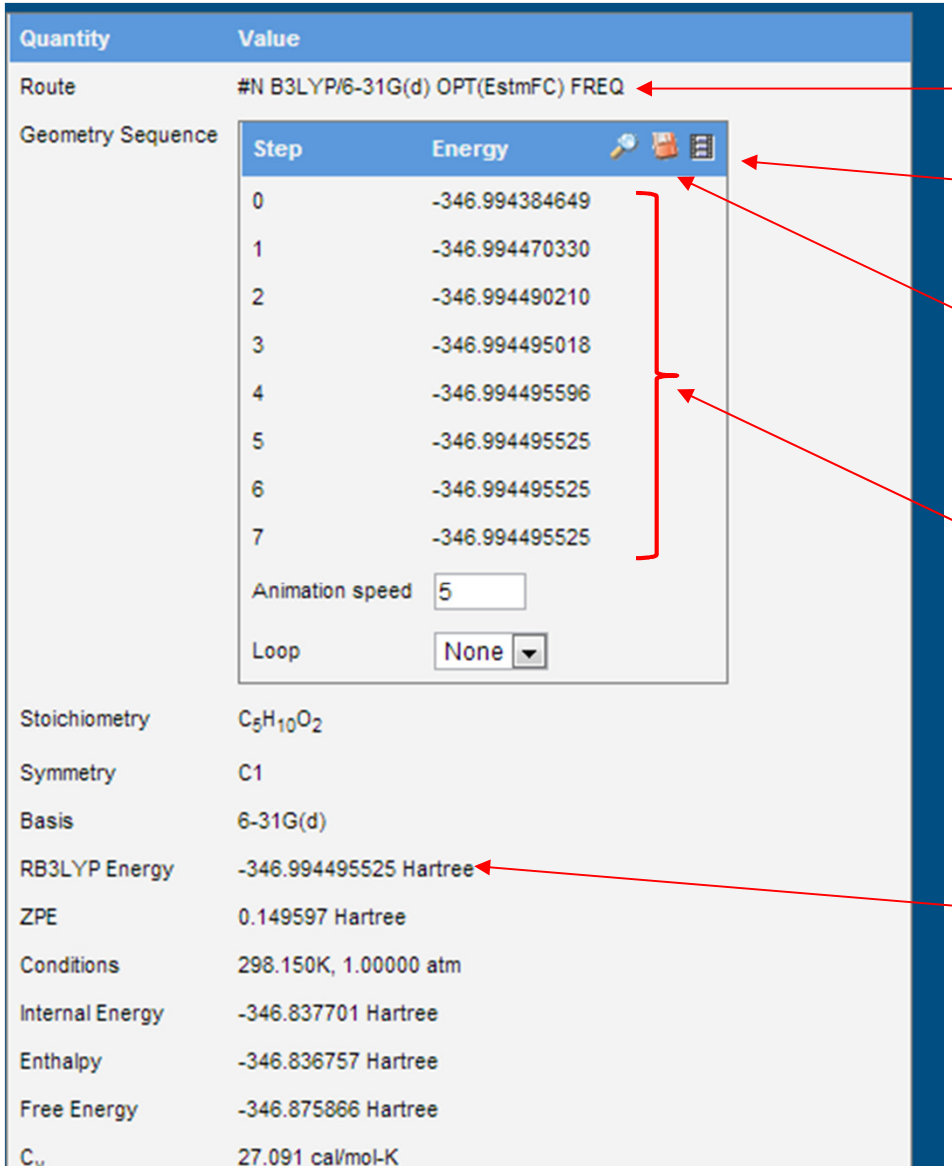
In the Job Manager window, you can view the results of a job finished or still running by clicking on the magnifying glass icon



- You will get a window showing the molecule like that shown to the left.
- don't forget to scroll down - there is lots more output.

Results

Shown below are the results below the 3D structure of the molecule that are a result of a geometry optimization.



Quantity	Value
Route	#N B3LYP/6-31G(d) OPT(EstmFC) FREQ
Geometry Sequence	

Step	Energy
0	-346.994384649
1	-346.994470330
2	-346.994490210
3	-346.994495018
4	-346.994495596
5	-346.994495525
6	-346.994495525
7	-346.994495525

Animation speed: 5

Loop: None

Stoichiometry	$C_5H_{10}O_2$
Symmetry	C1
Basis	6-31G(d)
RB3LYP Energy	-346.994495525 Hartree
ZPE	0.149597 Hartree
Conditions	298.150K, 1.00000 atm
Internal Energy	-346.837701 Hartree
Enthalpy	-346.836757 Hartree
Free Energy	-346.875866 Hartree
C_v	27.091 cal/mol-K

main Gaussian keywords

'movie' icon will show an animation of each geometry during the optimization

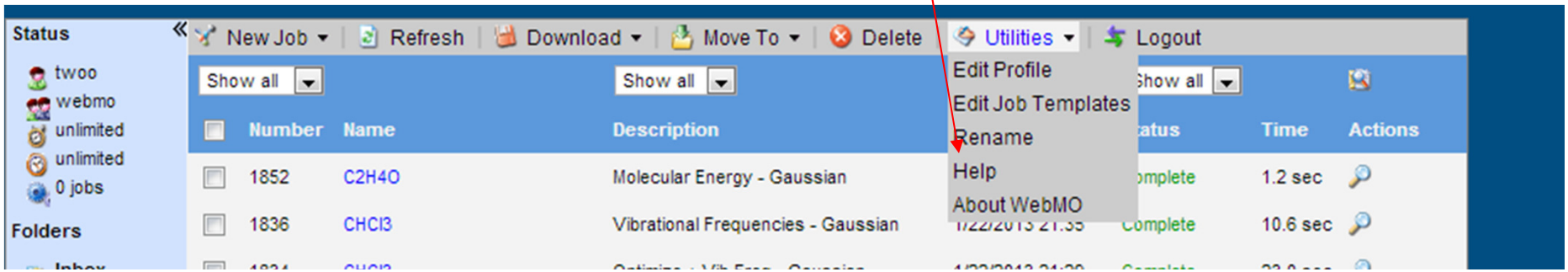
'disk' icon generally allows you to export results to a spreadsheet.

these are the energies of the system at each step of the geometry optimization.

the final total energy resulting from the geometry optimization. The units are in atomic units.

WebMO – Getting Help

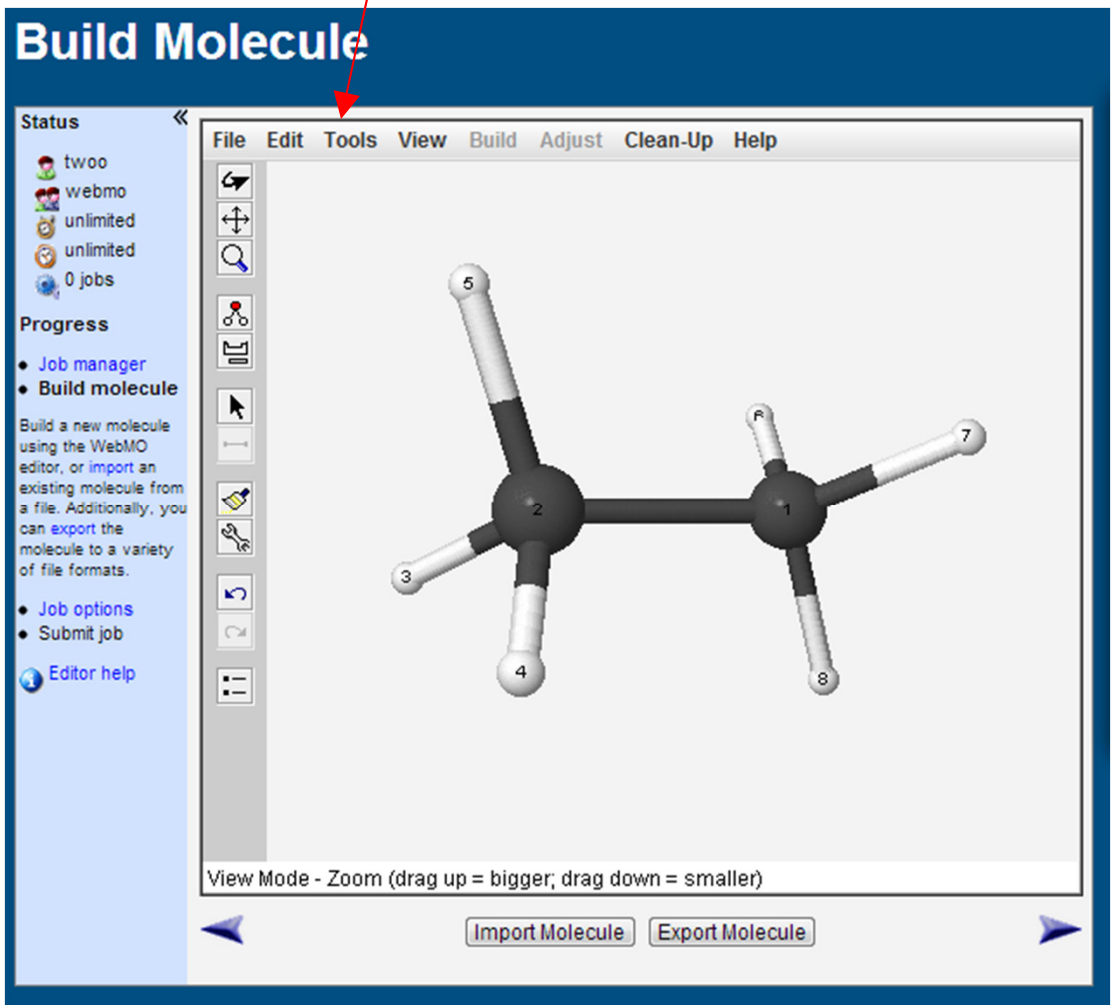
- WebMO has a help screen in the Utilities menu in the Job Manager



- One can go to the WebMO website for help at www.webmo.net.

How to Set Up a Coordinate Scan

- First build your molecule in the 'Build Molecule' window.
- In the 'Tools' drop down menu select the 'Z-matrix' editor.



One can use Cartesian coordinates to define the geometry of a system.

The Z-matrix of a molecule is an alternative way to define the geometry of a system.

In a Z-matrix atoms are one-by-one defined relative to previous atoms by a bond lengths, bond angles and bond dihedral angles.

The Z-matrix is often referred to as the 'internal' coordinates.

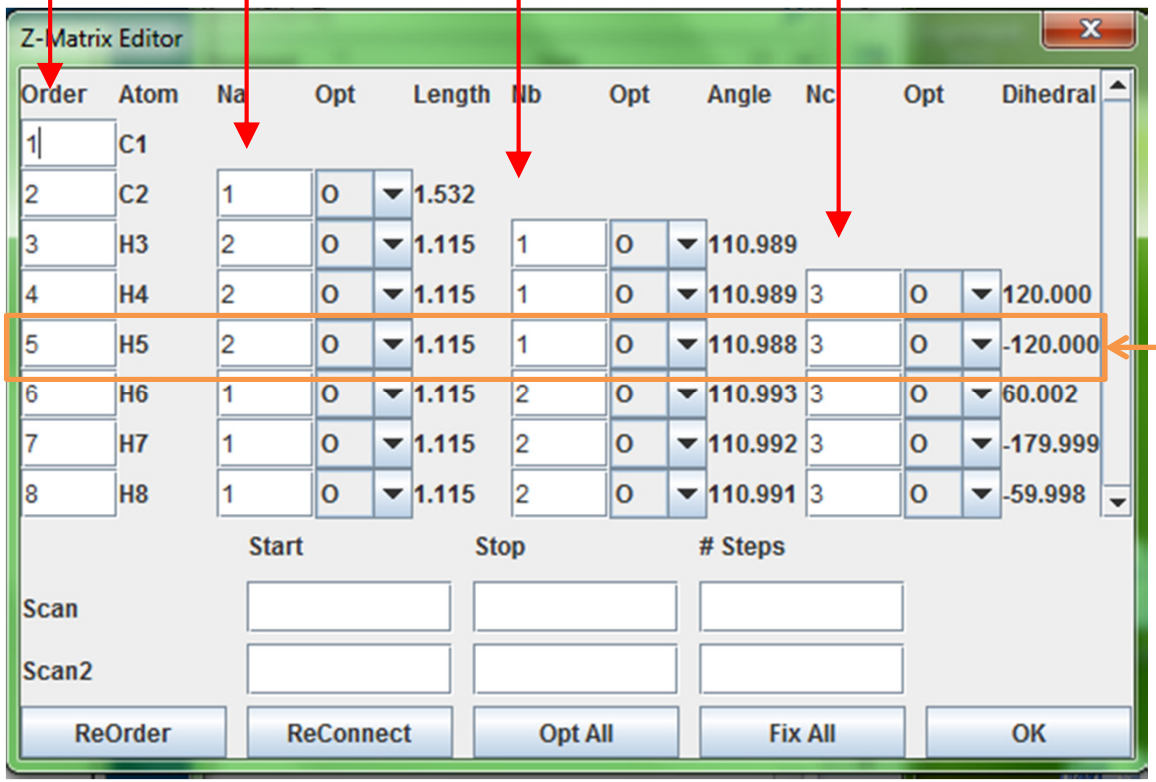
Understanding the Z-matrix Window

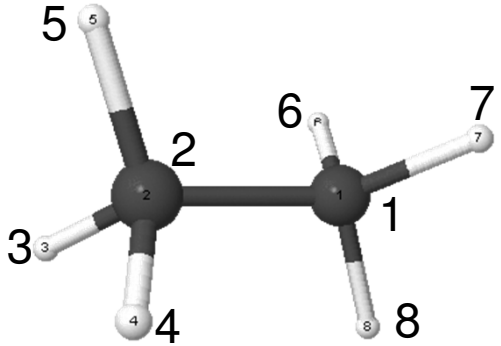
atom number

atom it forms bond with

atom it forms angle with (the 1st two atoms)

atom it forms a dihedral angle with





Consider the highlighted row:

atom '5' forms a bond with atom '2' that is 1.115 Å long

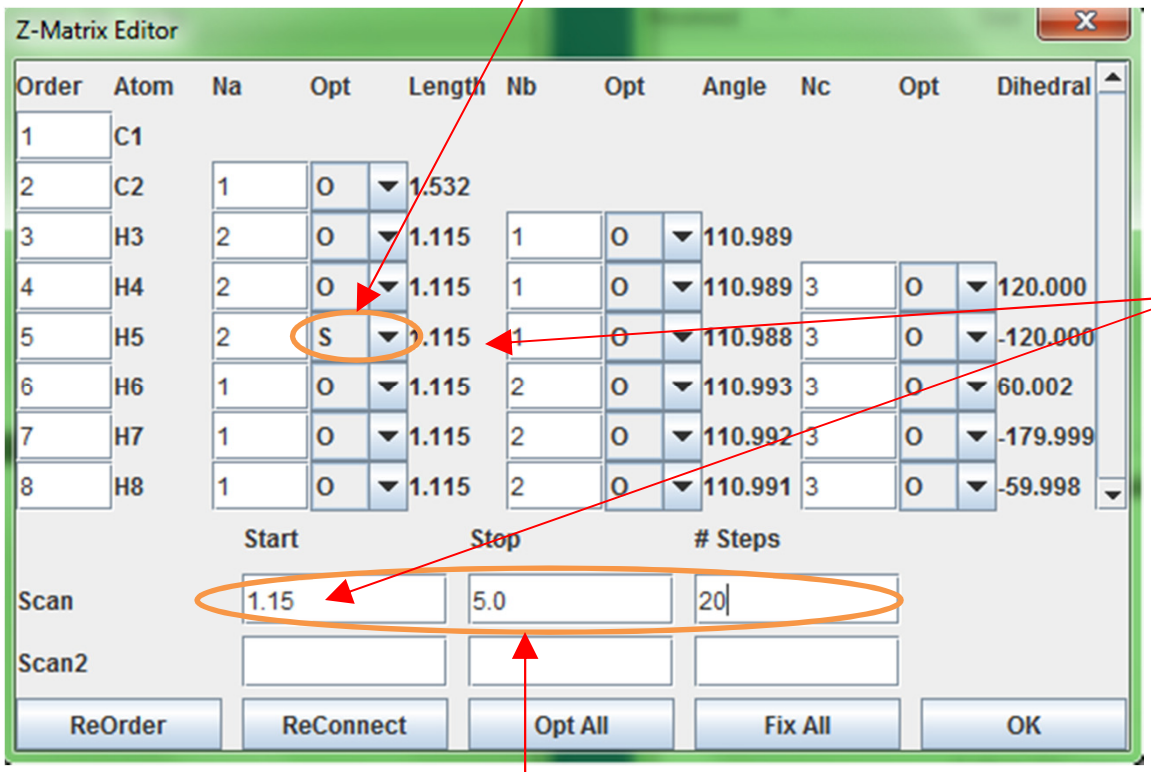
atoms '5' & '2' form a angle with atom '1' that is 110.993 degrees

atoms '5'-'2'-'1' form a dihedral angle with atom '3' that is -120 degrees

Setting Up Coordinate Scan in the Z-matrix Editor

Let us set up a coordinate scan to stretch the bond between atoms 5 and 2

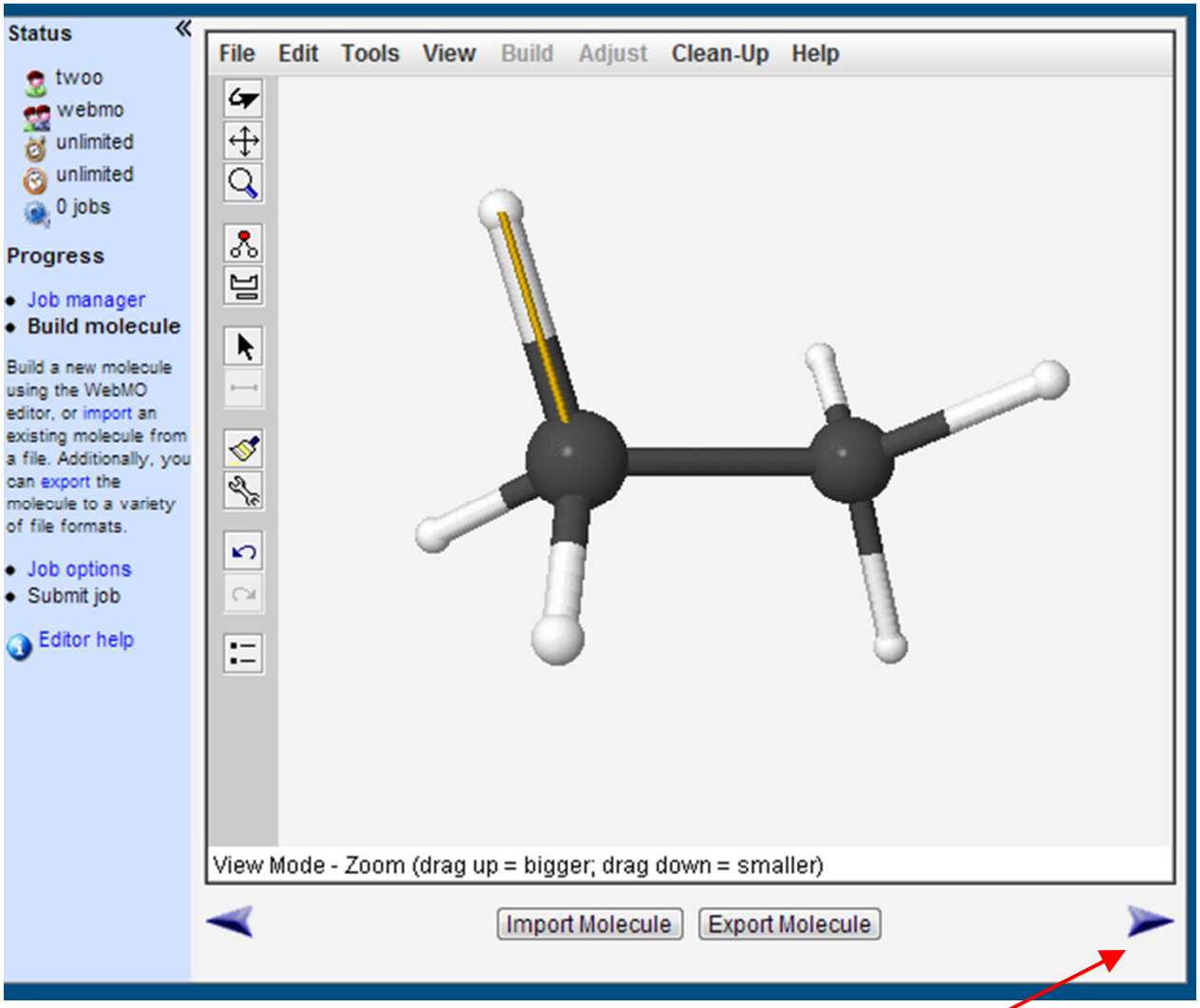
change the 'o' for optimize to 's' for scan.



It is best to use a starting value of the coordinate scan that is close to the current value.

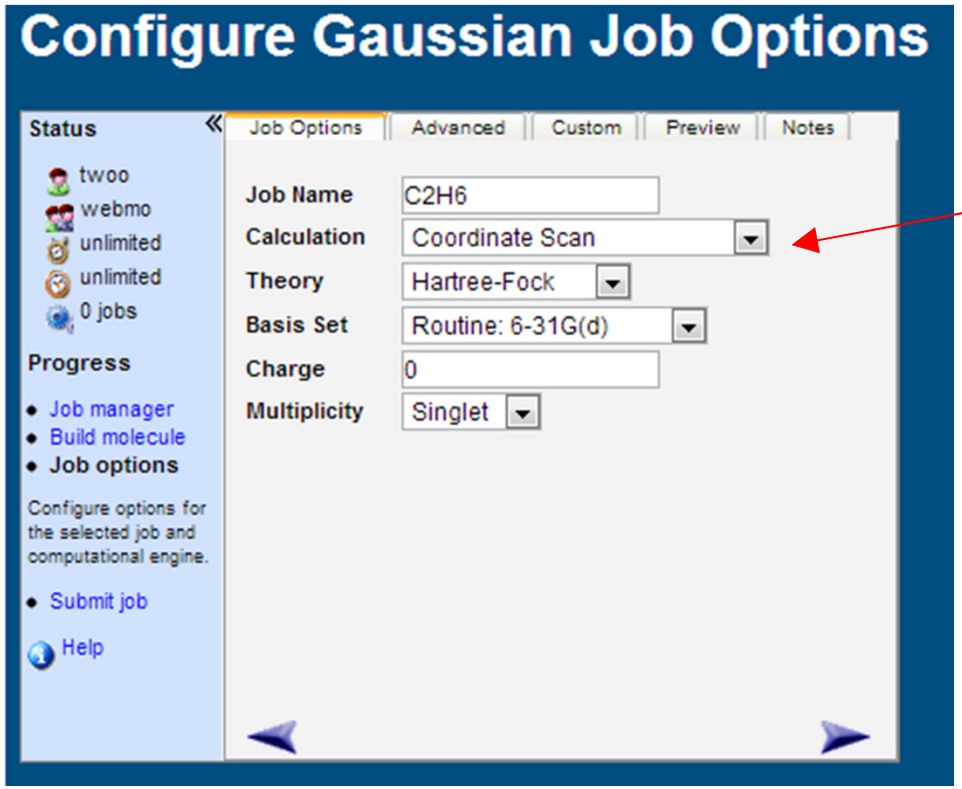
fill in these text boxes to start the scan at 1.15 Å and end at 5 Å in 20 steps.

After clicking 'Okay' in the Z-matrix editor window, the coordinate you want will be highlighted as shown below:



click this arrow to continue to the job configuration menu

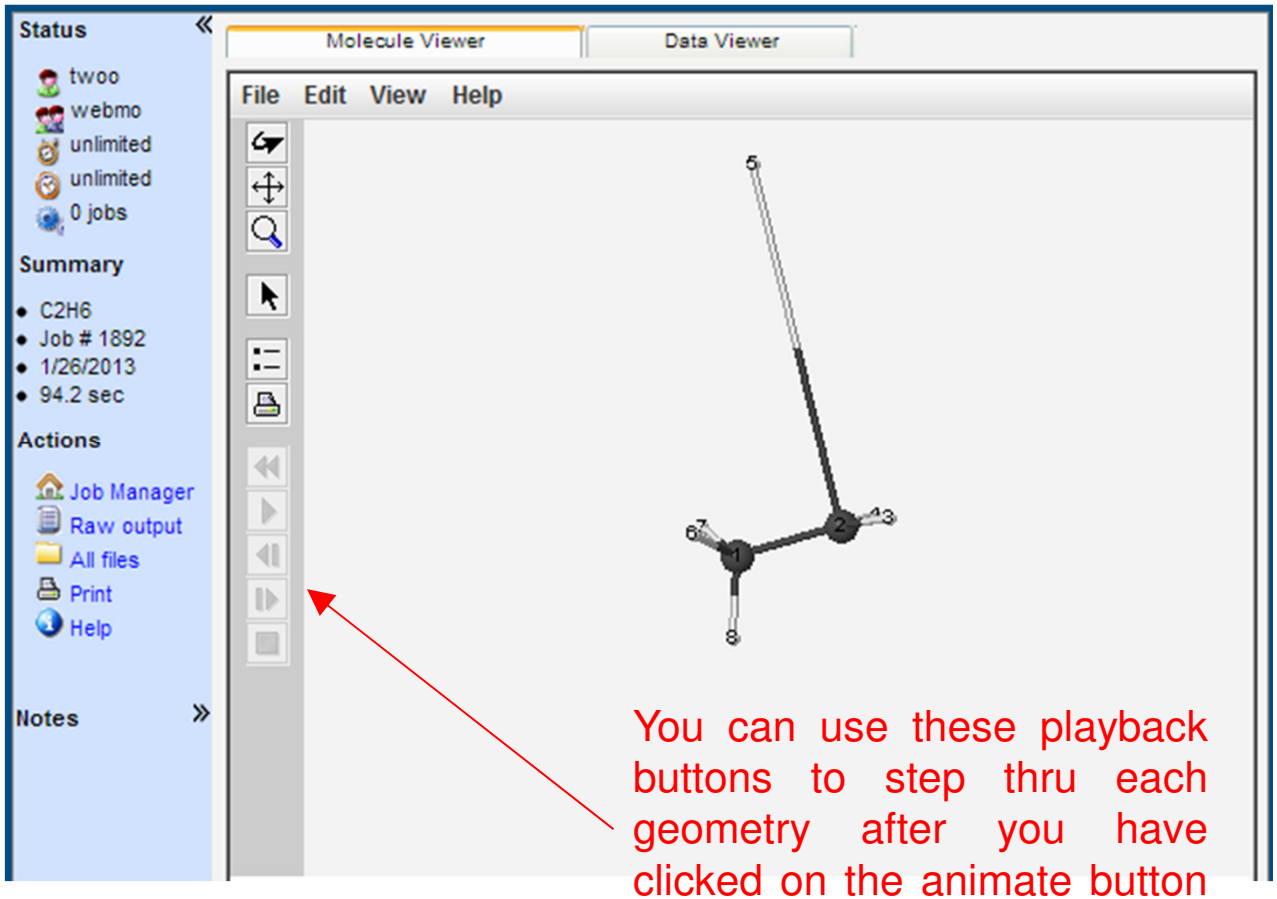
Coordinate Scan - Job Options



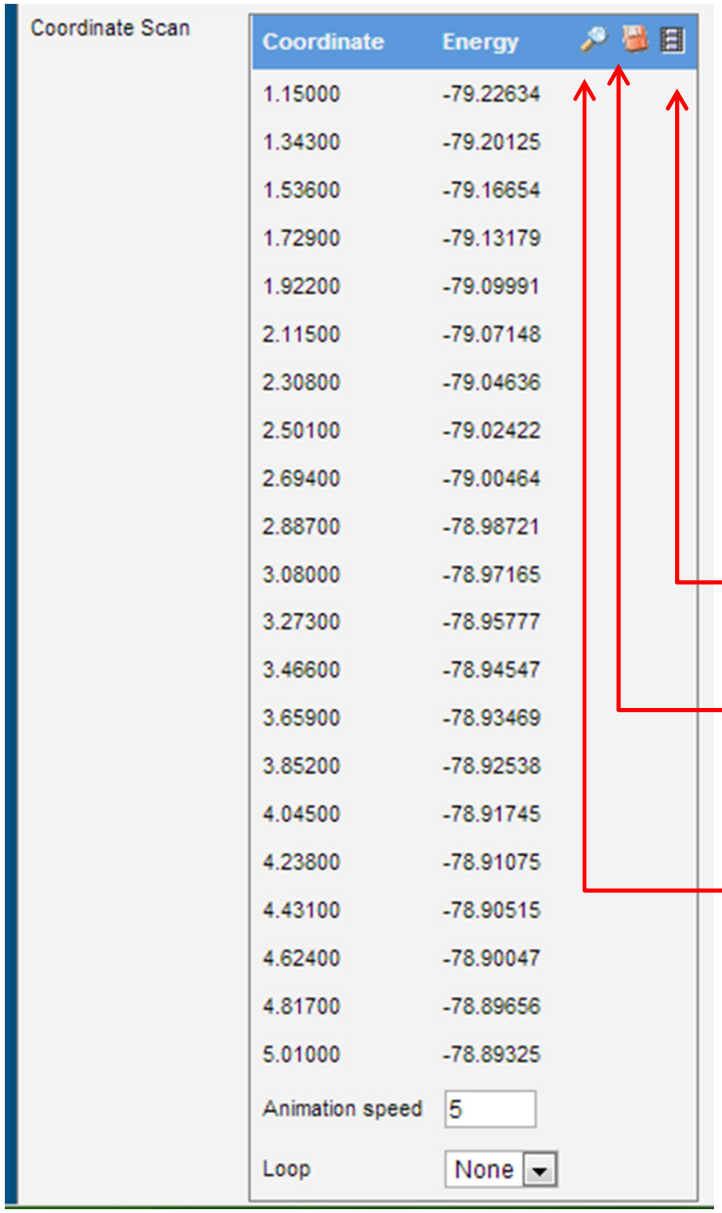
make sure the calculation type is set to 'Coordinate Scan'.

Coordinate Scan - Results

When the job is complete (and successful), the geometry shown will be the last one from the scan - in our example the C-H bond was scanned from 1.15 to 5.0 Å. Note that the system is depicted with the 'bonds' or connectivity of the originally drawn structure.



Coordinate Scan - Results



When the job is complete, the results window will show a 'Coordinate Scan' section.

It will show the coordinate and the energy of the system where the scan coordinate was fixed and all other coordinates were optimized.

will 'animate' the geometry through each step of the coordinate scan

save the data to your computer

show a plot