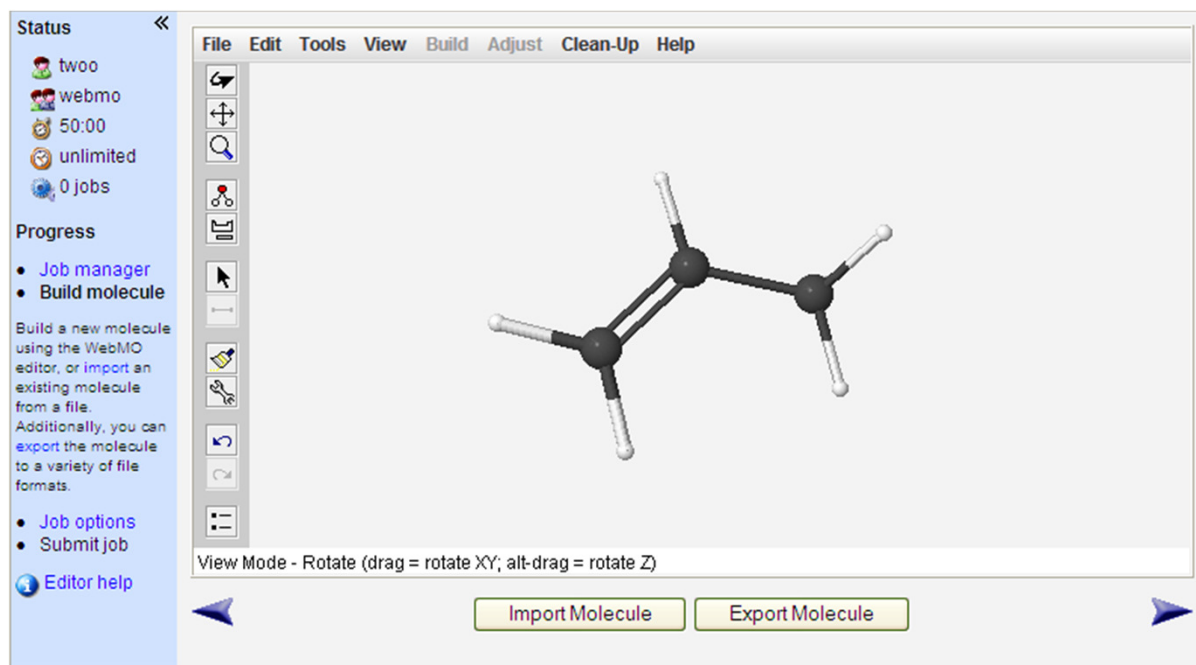


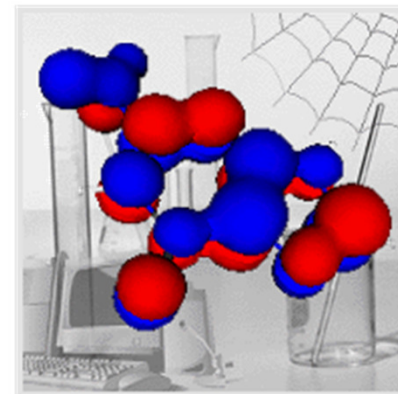
# Introduction to WEBMO



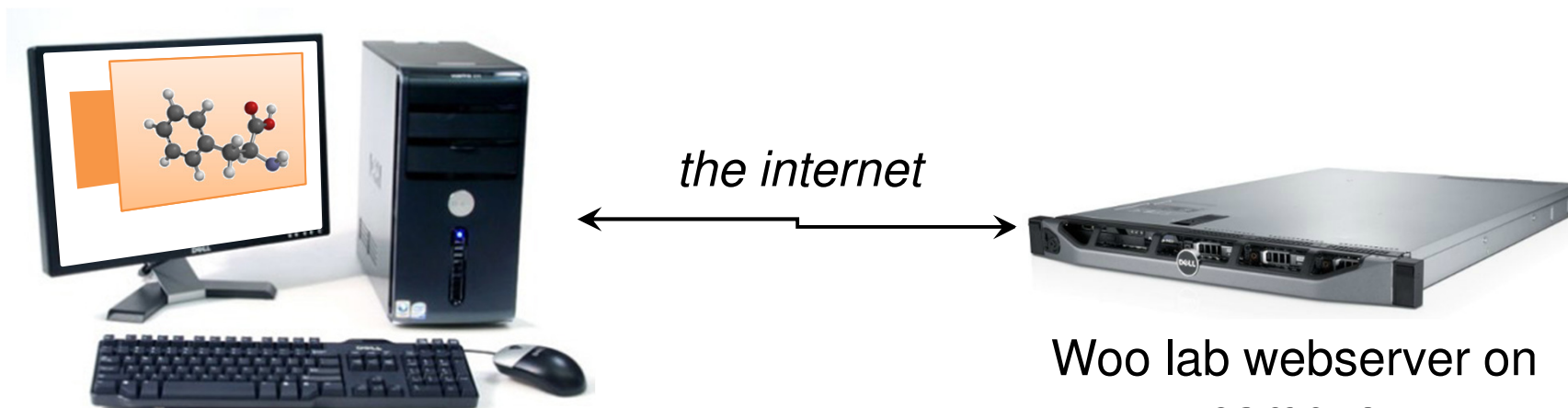
- WebMO is a web based graphical user interface to popular quantum chemistry packages like Gaussian.

Connect to WebMO Compu

- 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



### **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

**WebMO Job Manager**

Status: twoo, webmo, unlimited, unlimited, 0 jobs

Folders: Inbox, Trash

Search: Displayed jobs, Search

Navigation: New Job, Refresh, Download, Move To, Delete, Utilities, Logout

Number	Name	Description	Date	Status	Time	Actions
1852	C2H4O	Molecular Energy - Gaussian	1/23/2013 19:50	Complete	1.2 sec	
1836	CHCl3	Vibrational Frequencies - Gaussian	1/22/2013 21:35	Complete	10.6 sec	
1834	CHCl3	Optimize + Vib Freq - Gaussian	1/22/2013 21:29	Complete	23.0 sec	
1742	pentanone gas	Optimize + Vib Freq - Gaussian	12/8/2012 20:42	Complete	9:34	
1741	chain 4 b3lyp	Optimize + Vib Freq - Gaussian	12/8/2012 18:44	Complete	12:19	
1740	chain 3 B3lyp	Optimize + Vib Freq - Gaussian	12/8/2012 18:43	Complete	14:47	
1738	pentanone water	Optimize + Vib Freq - Gaussian	12/8/2012 18:19	Complete	16:12	
1737	pentanone cyclohexane	Optimize + Vib Freq - Gaussian	12/8/2012 18:16	Complete	17:14	
1736	chain 2 cyclohexane	Optimize + Vib Freq - Gaussian	12/8/2012 18:15	Complete	32:46	
1735	chain 2 water	Optimize + Vib Freq - Gaussian	12/8/2012 18:14	Complete	24:16	

# Web MO – Build Molecule Window

The screenshot shows the Web MO Build Molecule Window interface. On the left is a sidebar with a 'Status' section showing user 'twoo', 'webmo', a timer at '50:00', 'unlimited' status, and '0 jobs'. Below is a 'Progress' section with links for 'Job manager' and 'Build molecule', and a description of building a new molecule or importing an existing one. At the bottom of the sidebar are links for 'Job options', 'Submit job', and 'Editor help'. The main window has a menu bar with 'File', 'Edit', 'Tools', 'View', 'Build', 'Adjust', 'Clean-Up', and 'Help'. A toolbar on the left contains icons for various functions, with red arrows and text labels pointing to them: 'move, rotate, zoom' (pointing to the first three icons), 'build' (pointing to the fourth icon), 'change element' (pointing to the fifth icon), 'select tool' (pointing to the sixth icon, with a sub-note: '• hold shift or click and drag to select more than one atom'), 'clean up' (pointing to the seventh icon, with a sub-note: '• wrench is usually better'), 'undo/redo' (pointing to the eighth icon), and 'preferences' (pointing to the ninth icon). The main canvas displays a 3D ball-and-stick model of a molecule. A red arrow points from the text 'When molecule build is complet, click this button to continue' to a button in the bottom right corner. At the bottom of the window are 'Import Molecule' and 'Export Molecule' buttons. A status bar at the bottom left reads 'View Mode - Rotate (drag = rotate XY; alt-drag = rotate Z)'.

Status

twoo  
webmo  
50:00  
unlimited  
0 jobs

Progress

- Job manager
- Build molecule

Build a new molecule using the WebMO editor, or [import](#) an existing molecule from a file. Additionally, you can [export](#) the molecule to a variety of file formats.

- Job options
- Submit job

[Editor help](#)

File Edit Tools View Build Adjust Clean-Up Help

move, rotate, zoom

build

change element

select tool

- hold shift or click and drag to select more than one atom

clean up

- wrench is usually better

undo/redo

preferences

When molecule build is complet, click this button to continue

Import Molecule Export Molecule

View Mode - Rotate (drag = rotate XY; alt-drag = rotate Z)

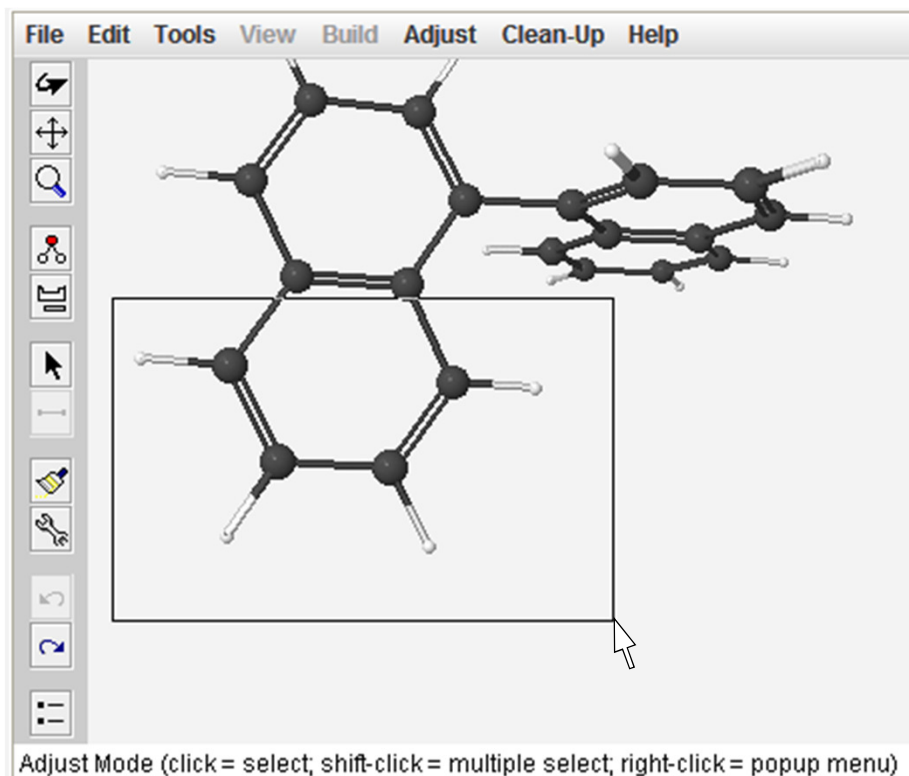
## Web MO – Molecule Building



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

Status

twoo  
webmo  
50:00  
unlimited  
0 jobs

Progress

- Job manager
- Build molecule

Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.

- Job options
- Submit job

Editor help

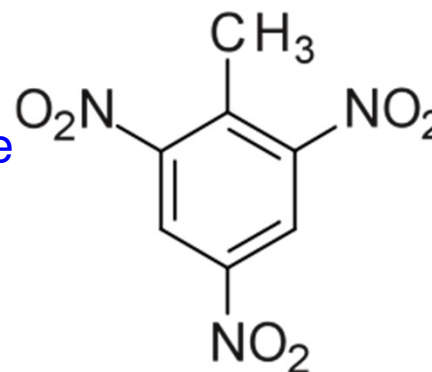
File Edit Tools View Build Adjust Clean-Up Help

To change the hybridization or formal charge right-click the atom with the select tool

View Mode - Rotate (drag = rotate XY; alt-drag = rotate Z)

Import Molecule Export Molecule

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

### WebMO Job Manager

The screenshot shows the WebMO Job Manager interface. On the left, there's a sidebar with 'Status' (twoo, webmo, 50:00, unlimited, 0 jobs) and 'Folders' (Inbox). The main area has a toolbar with 'New Job', 'Refresh', 'Download', 'Move To', 'Delete', 'Utilities', and 'Logout'. Below the toolbar is a table of jobs with columns: Number, Name, Description, Date, Status, Time, and Actions. The table contains three rows: 1813 (morphine - geometry opt, Running, 0.0 sec), 1810 (morphine - geometry opt, Complete, 2:54), and 1809 (BPP test, Complete, 37.3 sec). Red arrows point from the 'Refresh' button to the text 'Update the list', from the 'Delete' button to 'Kill or stop an active job', and from the 'Actions' column to 'View progress of job'.

Number	Name	Description	Date	Status	Time	Actions
1813	morphine - geometry opt	Geometry Optimization - Gaussian	3/1/2011 10:14	Running	0.0 sec	[Kill] [View]
1810	morphine - geometry opt	Geometry Optimization - Gaussian	3/1/2011 0:05	Complete	2:54	[View]
1809	BPP test	Geometry Optimization - Gaussian	2/28/2011 23:53	Complete	37.3 sec	[View]

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'

The screenshot shows the WebMO Job Manager interface with the 'Utilities' menu open. The menu options are: Edit Profile, Edit Job Templates, Rename, Help, and About WebMO. A blue arrow points from the 'Rename' option to the text 'To rename a job, select the job, then in the 'Utilities' menu click 'Rename''. Another blue arrow points from the 'Utilities' menu to the 'Rename' option. The table of jobs is visible in the background, with job 1809 (BPP test) selected.

Number	Name	Description	Date	Status	Time	Actions
1813	morphine - geometry opt	Geometry Optimization - Gaussian	3/1/2011 10:14	Running	19.1 sec	[View]
1810	morphine - geometry opt	Geometry Optimization - Gaussian	3/1/2011 0:05	Complete	2:54	[View]
1809	BPP test	Geometry Optimization - Gaussian	2/28/2011 23:53	Complete	37.3 sec	[View]
1808	C20H14	Geometry Optimization - Gaussian	2/28/2011 22:49	Complete	34.7 sec	[View]

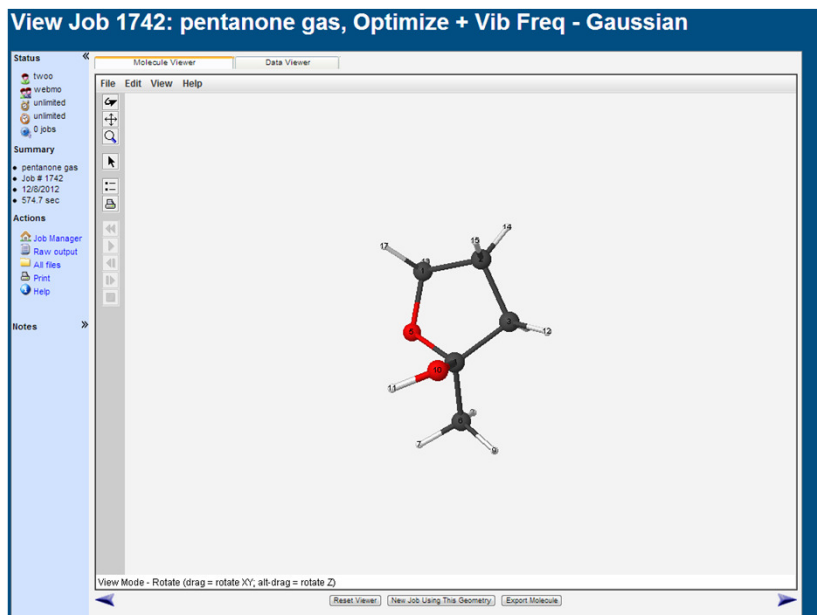


# How to View the Results of a Job?

## WebMO Job Manager

Number	Name	Description	Date	Status	Time	Actions
1813	morphine - geometry opt	Geometry Optimization - Gaussian	3/1/2011 10:14	Running	0.0 sec	[X] [Magnifying Glass] [Document]
1810	morphine - geometry opt	Geometry Optimization - Gaussian	3/1/2011 0:05	Complete	2:54	[Magnifying Glass]
1809	BPP test	Geometry Optimization - Gaussian	2/28/2011 23:53	Complete	37.3 sec	[Magnifying Glass]

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	<table><tr><th>Step</th><th>Energy</th></tr><tr><td>0</td><td>-346.994384649</td></tr><tr><td>1</td><td>-346.994470330</td></tr><tr><td>2</td><td>-346.994490210</td></tr><tr><td>3</td><td>-346.994495018</td></tr><tr><td>4</td><td>-346.994495596</td></tr><tr><td>5</td><td>-346.994495525</td></tr><tr><td>6</td><td>-346.994495525</td></tr><tr><td>7</td><td>-346.994495525</td></tr></table> <div>Animation speed <input type="text" value="5"/></div> <div>Loop <input type="text" value="None"/></div>	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
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																		
Stoichiometry	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>																		
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 <sub>v</sub>	27.091 cal/mol-K																		

main Gaussian keywords

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

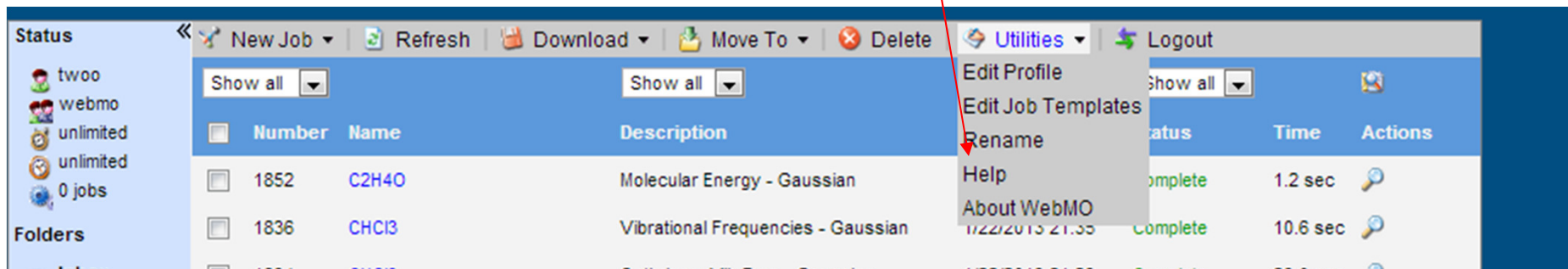
'disk' icon generally allows you to export results to a spreadsheet.

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

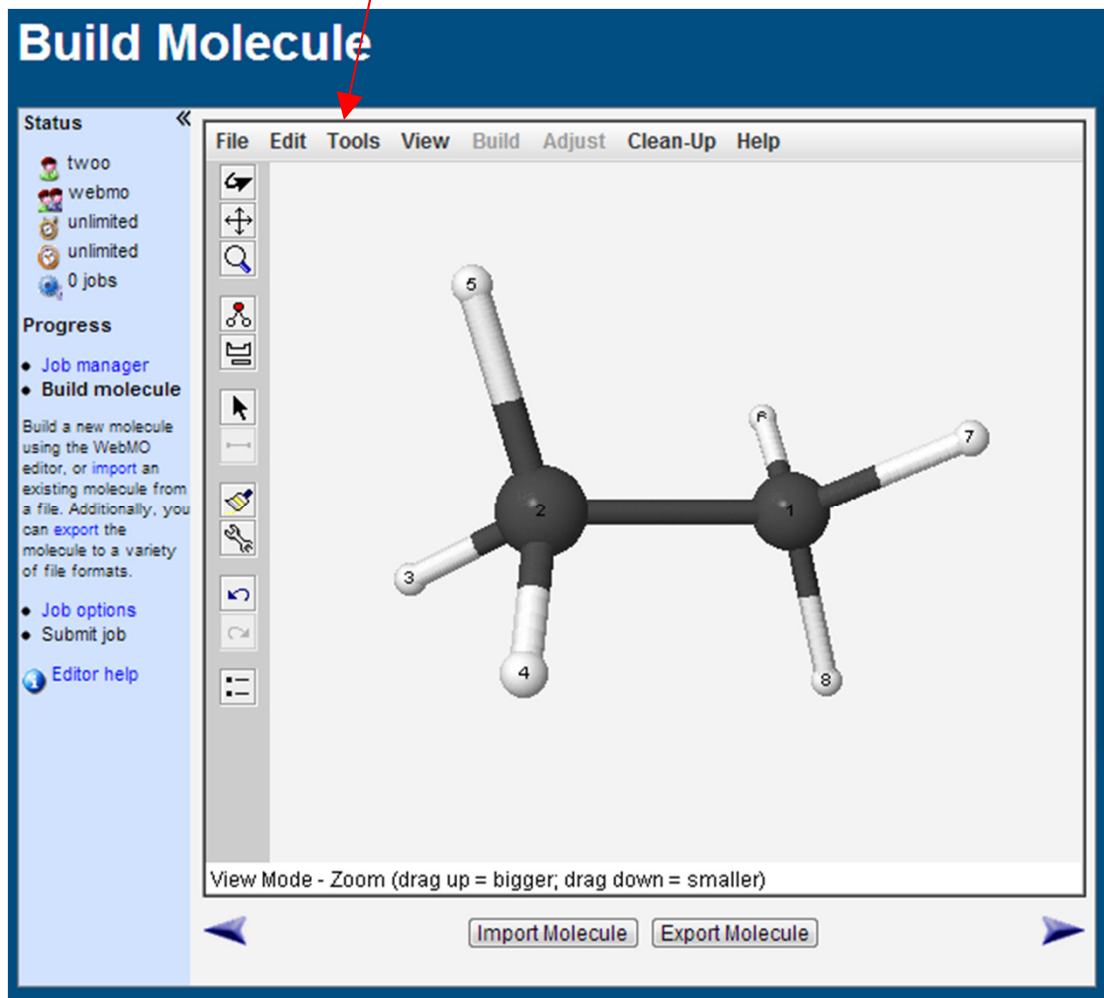
- WebMO has a help screen in the Utilities menu in the Job Manager



- One can go to the WebMO website for help at [www.webmo.net](http://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.



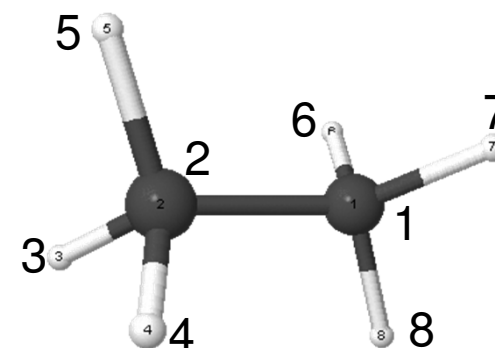
One can use Cartesian coordinates to define the geometry of a system.

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



Consider the highlighted row:

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

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

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

atom number

atom it forms bond with

atom it forms angle with (the 1<sup>st</sup> two atoms)

atom it forms a dihedral angle with

Z-Matrix Editor

Order	Atom	Na	Opt	Length	Nb	Opt	Angle	Nc	Opt	Dihedral
1	C1									
2	C2	1	O	1.532						
3	H3	2	O	1.115	1	O	110.989			
4	H4	2	O	1.115	1	O	110.989	3	O	120.000
5	H5	2	O	1.115	1	O	110.988	3	O	-120.000
6	H6	1	O	1.115	2	O	110.993	3	O	60.002
7	H7	1	O	1.115	2	O	110.992	3	O	-179.999
8	H8	1	O	1.115	2	O	110.991	3	O	-59.998

Start Stop # Steps

Scan

Scan2

ReOrder ReConnect Opt All Fix All OK

# 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.

The screenshot shows the Z-Matrix Editor window with a table of coordinates and a scan setup section. The table lists atoms and their coordinates, with the bond between atoms 5 and 2 highlighted. The scan setup section shows the start, stop, and number of steps for the scan.

Order	Atom	Na	Opt	Length	Nb	Opt	Angle	Nc	Opt	Dihedral
1	C1									
2	C2	1	O	1.532						
3	H3	2	O	1.115	1	O	110.989			
4	H4	2	O	1.115	1	O	110.989	3	O	120.000
5	H5	2	S	1.115	1	O	110.988	3	O	-120.000
6	H6	1	O	1.115	2	O	110.993	3	O	60.002
7	H7	1	O	1.115	2	O	110.992	3	O	-179.999
8	H8	1	O	1.115	2	O	110.991	3	O	-59.998

Start Stop # Steps

Scan 1.15 5.0 20

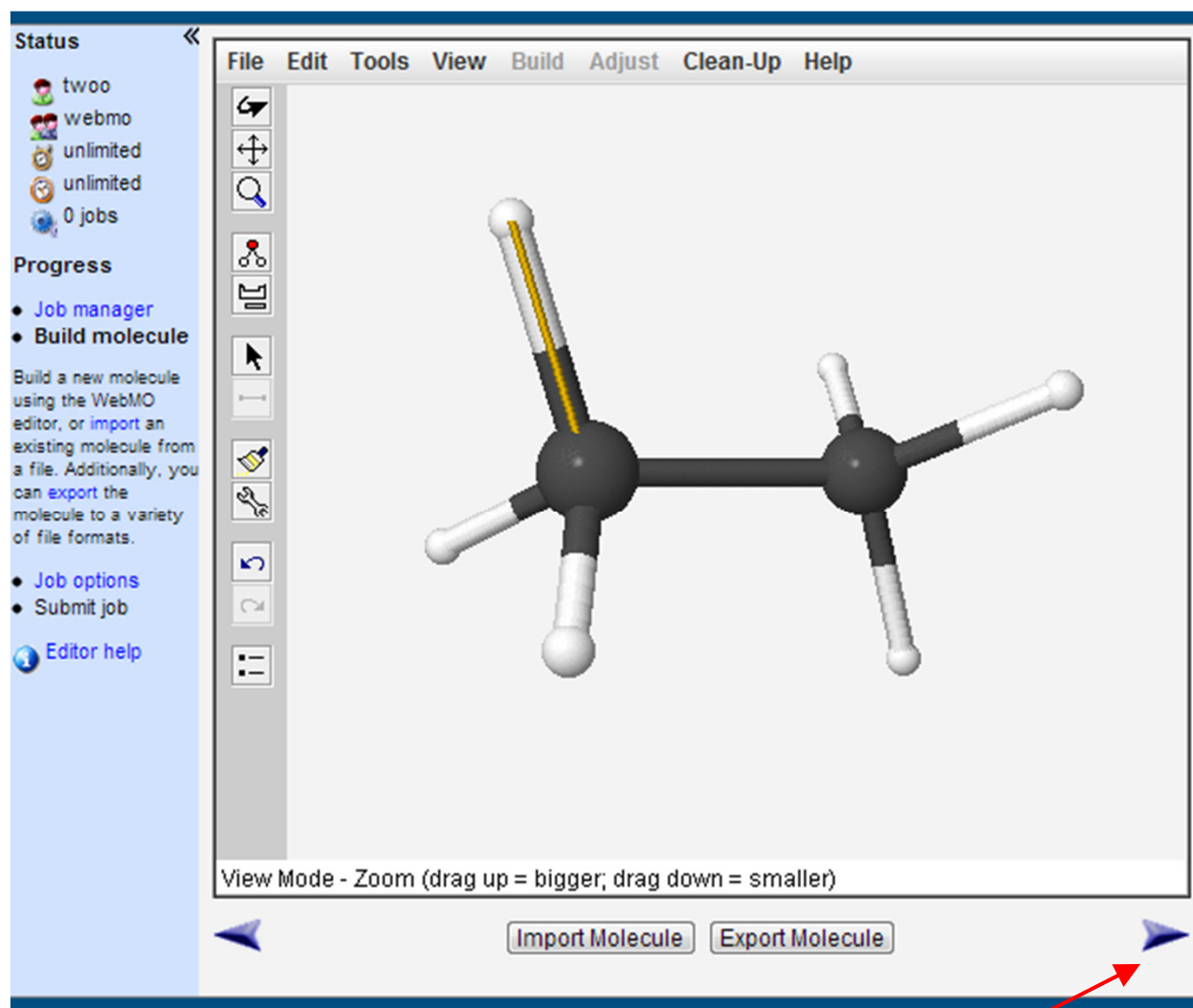
Scan2

ReOrder ReConnect Opt All Fix All OK

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

**Configure Gaussian Job Options**

Status << Job Options | Advanced | Custom | Preview | Notes

twoo  
webmo  
unlimited  
unlimited  
0 jobs

Progress

- Job manager
- Build molecule
- Job options

Configure options for the selected job and computational engine.

- Submit job

Help

Job Name: C2H6

Calculation: Coordinate Scan

Theory: Hartree-Fock

Basis Set: Routine: 6-31G(d)

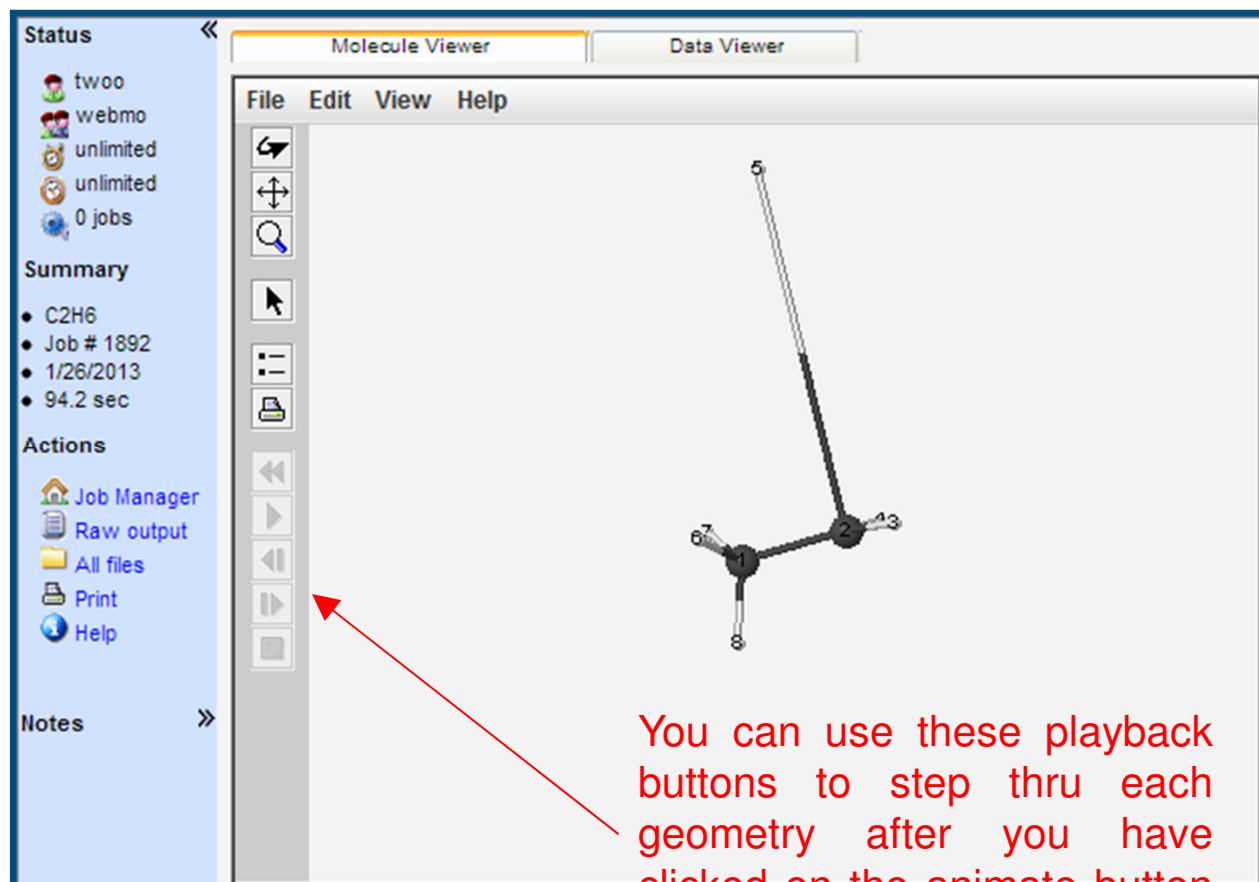
Charge: 0

Multiplicity: Singlet

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

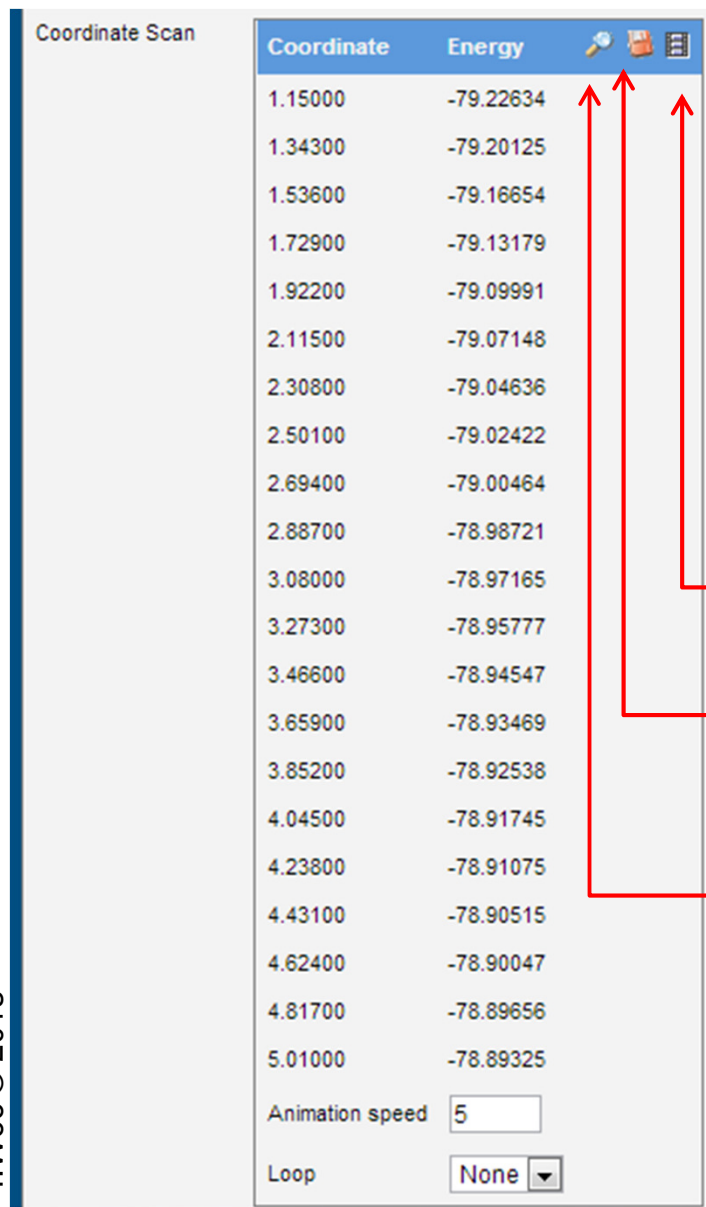
## Coordinate Scan - Results

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.



You can use these playback buttons to step thru each geometry after you have clicked on the animate button (see next slide)

## Coordinate Scan - Results



Coordinate	Energy
1.15000	-79.22634
1.34300	-79.20125
1.53600	-79.16654
1.72900	-79.13179
1.92200	-79.09991
2.11500	-79.07148
2.30800	-79.04636
2.50100	-79.02422
2.69400	-79.00464
2.88700	-78.98721
3.08000	-78.97165
3.27300	-78.95777
3.46600	-78.94547
3.65900	-78.93469
3.85200	-78.92538
4.04500	-78.91745
4.23800	-78.91075
4.43100	-78.90515
4.62400	-78.90047
4.81700	-78.89656
5.01000	-78.89325

Animation speed

Loop

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