WebMO User's Guide



WebMO User's Guide

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1. WebMO Introduction

A. Overview

WebMO is a web-based interface for computational chemistry programs. WebMO makes it possible to set up, run, and visualize **state-of-the-art chemical calculations** from any computer using **only a web browser**. WebMO is ideal for:

- Students who are learning and using computational chemistry
- Faculty who provide access to computational chemistry programs
- Bench chemists who need to complement their experimental work with calculations
- Theoretical chemists who manage multiple calculations and projects
- Managers who leverage their computational chemistry investment across the enterprise

WebMO's web-based interface is a modern, networked version of the traditional workstation graphical user interface to a computational chemistry program. The advantages of a web-based architecture are:

- Ease-of-use: A web browser interface is familiar and easy to use
- Versatility: One interface runs many computational chemistry programs
- **Cost savings**: Less expensive hardware is required
- Labor savings: Maintenance of one server is easier than multiple workstations

WebMO installs on any unix computer (Linux, OS X, AIX, Solaris, IRIX, Ultrix, BSD, etc.). After a one-time installation, WebMO is accessed and administered from a standard web browser on any kind of computer (Windows, Macintosh, unix).

And most importantly, WebMO is **FREE**. Thousands of chemists have downloaded and used WebMO. There is no risk to try WebMO for your computational chemistry needs!

B. Capabilities

WebMO supports the most popular computational chemistry programs including:

- Gamess: Versions 1998 and later
- Gaussian: Versions 94, 98, and later
- Mopac: Versions 6, 7, 93, 2000, 2002, and later

The specific computational jobs that can be run depend on the capabilities of the underlying computational chemistry program. Calculations that can be run and/or visualized include:

- Molecular energy
- Geometry optimization
- Transition state optimization

1. WebMO Introduction

- Saddle calculation
- Vibrational frequencies, spectra, and motions
- UV-VIS frequencies and spectra
- NMR frequencies and spectra
- Thermochemistry
- Molecular orbitals and electron density isosurfaces
- Electrostatic potentials
- Nucleophilic and electrophilic frontier orbital densities
- IRC calculation
- Coordinate scan

C. Quickstart Tutorial

Login

For you to run WebMO, your system administrator will have established a WebMO user account for you and have provided you with a username and password.

Start your web browser, and type in the location of your WebMO implementation. The URL will be something like

http://server.domain.edu/~webmo/cgi-bin/login.cgi

Enter your Username and Password on the WebMO Login page and click Login. You will enter the Job Manager page.



WebMO Login Page

Job Manager

After logging in, you will be on the WebMO Job Manager page. This page displays your account information (username and compute time limits), the number of currently queued jobs, and a list of jobs you have submitted and/or run.

Click Create New Job near the bottom of the page to start a new job.

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obs Queued		0					
	1003 - 1110	Show all	Show all	Show all V		Filter	
Number 1	Name	Show all I	Show all 💽 Date	Show all	Time	Filter Actions	
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Number 1 15 ; 16 ; Select All	Name phenol para-quinone	Show all Description Optimize + Vib Freq - Gaussian Geometry Optimization - Gamess	Show all Image: Comparison of the second secon	Show all 💌 Status Complete Running	Time 1:40 32 sec	Filter Actions View Kil	en e

WebMO Job Manager Page

Build Molecule

The Build Molecule page allows you to draw the 3-D chemical structure for which you wish to perform calculations. Initially the display in the page will be blank, indicating that no molecule has been drawn. A navigation bar at the bottom of the page describes your progress in building the molecule, choosing a computational engine, setting job options, and submitting your job.

Click Open Editor to invoke the 3-D molecular editor and build a molecule.

1. WebMO Introduction

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	Job Manager	Build Molecule	Choose Engine	Job Options	Submit Job	
Done					👩 Internet	•

WebMO Build Molecule Page

Editor

The WebMO Editor has 3 tools:

- View: rotate, translate, or zoom molecule
- Build: add new atoms, bonds, or fragments
- Adjust: change bond lengths, bond angles, or dihedral angles

IMPORTANT TIP: The status line at the bottom of the Editor indicates the current tool and the editing operations that are possible.

To build a new molecule, choose **Tools**: Build (or click a on the toolbar) to start the build tool. The status line indicates the current atom, which is initially carbon. Add an atom by clicking. Add a bond and an atom by clicking on an existing atom and dragging. Add a bond by dragging between two existing atoms. To make a multiple bond, drag again between the atoms. To use a different atom, choose Build: O, Build: N, or Build: Other... (E). There is no need to add hydrogen atoms, as the WebMO Editor can do this automatically for you.

To adjust the viewpoint of the molecule, change to the view tool with Tools: View (or click one of the view tool buttons). Then choose View: Rotate (), View: Translate (), or View: Zoom (). Click and drag the mouse as indicated on the status line to rotate, translate, or zoom the molecule.

Missing hydrogens can be added and the molecular geometry can be idealized automatically by choosing Clean-Up: Comprehensive (

To further adjust the geometry (bond length, bond angle, or dihedral angle) of the molecule, choose Tools: Adjust (\blacktriangleright) to start the adjust tool. Select 2, 3, or 4 atoms by clicking the first atom and shift-clicking all subsequent atoms. Then choose Adjust: Bond Length (\boxdot), Adjust: Bond Angle (\bigtriangleup), or Adjust: Dihedral Angle (\boxdot), respectively. Enter the new desired value into the dialog box and click OK. Note that the first atom that was selected is the atom that is moved.

An online tutorial for the WebMO Editor is available by choosing Help and scrolling down to the Tutorial section.

After the molecule has been built, choose File: Close to return to the Build Molecule page. The molecule will appear on the display in the page.

Click Choose Engine to select the computational engine you will use to perform your calculation. (If only one computational engine is available, the Choose Engine option is not present. Instead, choose Job Options and continue at the corresponding section below.)



WebMO 3-D Molecular Editor

Choose Computational Engine

The WebMO interface supports the following computational chemistry programs:

- Gamess: *ab initio* and semi-empirical calculations (free)
- Gaussian: *ab initio* and semi-empirical calculations (commercial)
- MOPAC: semi-empirical calculations (free)

These programs must be installed separately by the system administrator (see http://www.webmo.net/support for instructions).

1. WebMO Introduction

If more than one program is installed, choose which program to use. If the program is available on multiple computers, select the desired server. Click Job Options to continue.

If only one computational chemistry program is installed then this page is skipped.

Choo	se Computatio	nal Engine	•
Engine	Description		
© Gamess	Ab initio and semi	-emperical calculation	15
• Gaussian	Ab initio and semi	-empirical calculations	5
C Mopac	Semi-empirical ca	lculations	
Select Serve	r www.webmo.net 💌]	1 /

WebMO Choose Computational Engine Page

Configure Job Options

The details of the Configure Job Options page depend on the specific computational engine chosen. In general, however, you will be able to:

- Enter a Job Name, i.e., an arbitrary name describing the calculation
- Specify the Calculation type, e.g., Geometry Optimization or Molecular Orbitals
- Select a level of Theory, e.g., Hartree-Fock
- Select a Basis Set, e.g., 6-31G(d)

You may also specify the overall Charge and Multiplicity of the molecule.

The Advanced Options button gives you access to less commonly used options, e.g., the specification of additional keywords.

If you wish to view and optionally edit the actual input file being submitted to the computational chemistry program, check the **Preview Input File** box.

After entering the job name, calculation type, level of theory, and basis set, click Submit Job to send the job to WebMO's queue. (If Preview Input File was checked, click Submit Job on the page displaying the input file.)

Co	onfigure Ga	nussian Jo	b Option	15
	Job Name			
	Calculation	Single Point	•	
	Theory	Hartree-Fock		
	Basis Set	Basic: 3-21G	•	
	Charge	0		
	Multiplicity	Singlet 💌		
	Preview Input File			
	Advanced Optic	ns		
<u>Job Manager</u>	Build Molecule	<u>Choose Engine</u>	Job Options	<u>Submit Job</u>

WebMO Configure Job Options Page

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	Additional Keywords	

WebMO Advanced Options Page

Job Manager

Jobs submitted to WebMO are queued and then run at the first available opportunity. If no other jobs are currently queued or running, the submitted job will be run immediately.

The Job Manager page will display the status of your submitted jobs as: Queued, Running, Completed, or Failed. Click the **Refresh** button on the bottom on the page to update the status of your jobs.

The amount of CPU time spent on a job is displayed, so that you can monitor how long your job has been running. You may also view the output file of a running job by clicking the **Raw Output** button.

1. WebMO Introduction

If necessary, you may terminate a queued or running job by clicking the Kill button. Jobs that exceed a user's compute time limits are automatically terminated.

When the job is finished, the status will either be Completed or Failed, depending on the whether the underlying program was able to complete the requested calculation. To view the results of a completed calculation, click the View button. If the calculation failed, click the Raw Output button to determine the reason for failure, which is usually indicated near the end of the output file.

/cbl	<mark>40 Job Mar</mark> Edit <u>V</u> iew	a <mark>ger - Microsoft Inter</mark> F <u>a</u> vorites <u>T</u> ools <u>H</u> e	net Explorer					
va	ilable	Jobs - Inbox	99					6
			Show all	Show all 💌	Show all 💌		Filter	
	Number	Name	Description	Date	Status	Time	Actions	
-	15	phenol	Optimize + Vib Freq - Gaussian	11/15/2002 13:43	Complete	1:40	View	
-	16	para-quinone	Geometry Optimization - Gamess	11/15/2002 13:46	Complete	2:36	View	
-	17	acetamide cation	Geometry Optimization - Gaussian	11/15/2002 13:52	Failed	0.9 sec	Raw Output	Restart
1	18	acetamide	Geometry Optimization - Gaussian	11/15/2002 13:57	Running	39 sec	KI	Raw Output
-	19	formyl fluoride	Geometry Optimization - Mopac	11/15/2002 13:57	Queued (1/1)	0 sec	KI	
-	Select Al	1						
De	lete D	ownload Renam	e Spreadsheet		Folders M	ove To	-Move to Selec	ted Folder- 💌
efn	esh 🛛 🔿	Create New Job	Import Job Edit Profile Abo	out WebMO	Logout			
one								Internet

WebMO Job Manager with Completed, Failed, Running, and Queued Jobs

View Job

At the top of the View Job page is a display of the molecule's geometry, which can be rotated, translated, and zoomed using the toolbar buttons as described above in the Editor section. Selecting 2, 3, or 4 atoms will display the corresponding bond length, bond angle, or dihedral angle.

The remainder of the View Job page depends on the specific computational engine and calculation type. Information that can be displayed includes:

- Energy
- Rotational Constants
- Dipole Moment
- Partial Charges
- Bond Orders
- Vibrational Modes
- Molecular Orbitals
- NMR Shifts

and other information.

Clicking on a View button can graphically display:

- Dipole Moment
- Partial Charges
- Normal Modes
- Infrared Spectrum
- UV-Vis spectrum
- NMR Spectrum

A new job may be started using the final geometry of the current calculation by clicking New Job Using This Geometry.

The final geometry may be exported into a variety of formats using the Export Molecule button.

The complete output file of the computational chemistry program may be viewed by clicking the Raw Output button.



WebMO View Job Page (part 1/2)

1. WebMO Introduction

	lantiti	es						
Quantity	Value							
Route	PM3 BC	NDS CH	ARGE=0	SINGLET				
Symmetry	CS							
Heat of Formation	-88.7980	i3 kcal/m	ol					
Dipole Moment	2.449 E	ebye 🔵	View					
Partial Charges					ĩ			
Ť	Atom	Symbol	Charge	View				
	1	С	.3518					
	2	0	3096					
	3	F	1497					
	4	Н	.1075					
Bond Order	Atom	S	mbol	C	-	R	H	
	1	 C		3.463329		•		
	2	0		1.941851	10.527764			
	3	F		.958313	.119915	13.195342		
	4	Н		.932955	.029636	.025849	.796528	
Server	101010 100	hmo net						
0071	0.2	omomer						

WebMO View Job Page (part 2/2)

D. WebMO Pro

WebMO Pro is a commercial add-on to the freeware WebMO computational chemistry package. It features a variety of powerful enhancements that are suitable for advanced education, research-level, or commercial users.

In addition to the normal WebMO features, WebMO Pro adds the following:

- Support for remote computational servers
- Visualization of molecular orbitals
- Visualization of electron density and electrostatic potential
- Visualization of nucleophilic and electrophilic frontier orbital density
- · Improved job organization with user-customizable folders
- Creation of spreadsheet summaries to compare results from multiple jobs
- Integrated Z-matrix editor
- 1-D coordinate scanning
- Listing, viewing, and downloading of all input and output files
- Job calculation templates for individual users

Additional information about the capabilities of WebMO Pro is available at http://www.webmo.net/pro.

A. Using Existing Structures

Importing Structures

The first step in running a computational chemistry job is to specify the molecular structure for which the calculation should be performed. Sometimes a structure will already exist, e.g., on the web, in a database, or as a previous calculation. At other times, the user will have to create the structure (see next section).

Many molecular structures are already available as files or web documents in a variety of formats. WebMO allows one to import existing molecules in a variety of formats:

- MOL format
- PDB format
- XYZ format

or from a pre-existing input file:

- Gaussian (Z-matrix or cartesian)
- Mopac (Z-matrix or cartesian)

To import an existing structure, first save the desired molecular structure as a text file on your local hard disk. You might have another program that can generate and save molecular structures. You might download molecular structure files from the WWW. Or you might have old computational chemistry input files. Whatever the source of the molecular structure, it needs to be one of the above supported formats and should be saved on your hard disk.

A very useful source for obtaining, viewing, and saving common molecular structures is the Chime molecule viewer (available from MDL Information Systems. Inc. at http://www.mdlchime.com). There are many repositories of molecular structures in Chime format on the WWW (use any search engine to search for the terms like "chime" and "molecule"). To view and download these structures, the Chime plug-in must be installed on your computer. While viewing a molecular structure in Chime, right-click, choose File: Save Molecule As..., and save the molecule to disk either in PDB or in MOL format



Save Molecul	le File As				? ×
Save in: 🔁	Web Molecules	•	E	1 🖻	
aspirin.mol sucrose.mo taxol.mol	k				
, File <u>n</u> ame:	phenylalanine.mol				<u>S</u> ave
Save as type:	MDL Mol File Format Brookhaven Protein Data B	ank (PDB)	•		Cancel //
	MDL Mol File Format				

Using Chime to Save a Molecule to Local Disk

Once a molecule is saved to the local hard disk, it can be imported into WebMO. From the WebMO Job Manager page, click the Create New Job button (<u>Create New Job</u>) near the bottom of the page to reach the Build Molecule page. Click the Import Molecule button (<u>Import Molecule</u>) to bring up the Import Molecule dialog box. Choose the format of the saved file from the drop-down menu, click the Browse button and open the saved file, and click the Import Molecule button to complete the process. The imported molecule will be displayed on the Build Molecule page. If the structure is appropriate, proceed to the Choose Engine step (or Job Options step if only one computational engine is available). If you wish to modify the structure, click Open Editor to edit the structure.



Import Molecule from Local Disk into Web $M\overline{O}$

Some file formats lack bonding information or do not correctly indicate multiple bonds. In such cases, check the **Generate Bonds** box for WebMO to automatically generate bonds of the imported structure using simple distance relationships. It is wise to then check the structure and possibly open the editor to make any necessary changes.

When importing a molecule, it is possible to skip the step of saving the structure to the local hard disk. Simply copy and paste the structure information into the textbox in the Import Molecule page. The pasted text may be edited prior to clicking the Import Molecule button.

Structures from Previous WebMO Jobs

Sometimes one wishes to perform a calculation on the result of a previous WebMO job. For example, to compute the infrared spectrum of a molecule, one first optimizes the geometry of the molecule and then computes the vibrational frequencies of the optimized structure.

From the WebMO Job Manager page, scroll to the previous job, and click its View button (View). Near the top of the results page is a picture of the previously computed molecule. Click the New Job Using This Geometry button (<u>New Job Using This Geometry</u>) under the molecule. The Build Molecule page is opened displaying the molecule in its previously computed geometry. Do not open the WebMO Editor (unless you wish to modify the geometry). Simply proceed to the Choose Engine step (or Job Options step if only one computational engine is available).

If desired, the displayed molecular geometry can be verified prior to running a job by clicking the Select button (\blacktriangle). Select two, three, or four atoms by clicking the first atom and shift-clicking subsequent atoms. The corresponding bond length, bond angle, or dihedral angle is reported on the status line. When investigating the geometry of a molecule, it may be useful to reorient the displayed molecule, which can be done by clicking the rotate (\boxdot), translate (\boxdot), or zoom (\boxdot) buttons and the dragging the molecule appropriately with the mouse.

B. WebMO Editor

WebMO contains a built-in 3-D molecular editor to create molecular structures for use in subsequent calculations.

From the WebMO Job Manager page, click the **Create New Job** button (<u>Create New Job</u>) near the bottom of the page to reach the Build Molecule page. Click the **Open Editor** button (<u>Open Editor</u>) to invoke the 3-D WebMO molecular editor. The WebMO Editor opens in a separate window.

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File	Edit	Tools	View	Build	Adjust	Clean-Up	Help		
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I									
Q									
8									
님									
1									
5									
View	Mode	- Rotate	(drag =	rotate	XY; ctrl-c	Irag = rotate	Z)	 	
Warn	ing: Ap	oplet Wi	ndow						

WebMO 3-D Molecular Editor

All features of the WebMO Editor are available from the menu along the top of the editor window. The most common operations are also available on the toolbar along the left side of the window. The status line at the bottom of the window offers continuous help on currently permitted operations.

The WebMO Editor has 3 tools (or modes of operation):

- View: rotate, translate, or zoom molecule
- Build: add new atoms, bonds, or fragments
- Adjust: change bond lengths, bond angles, or dihedral angles

The active tool is indicated both on the menu and on the status line.

Use of the mouse in the WebMO Editor is very intuitive. One inserts atoms and draws bonds by clicking and dragging the mouse. One also moves the mouse in a natural fashion to rotate, translate, and zoom the molecule. A complete list of WebMO Editor actions is given in the following table, as well as described in subsequent sections.

Tool	Action	Description
Build	Click	Add current atom (or fragment)
	Click on atom and drag	Add bond and current atom
	Drag between atoms	Add bond
	Multiple drag between atoms	Change bond order
	Build: Other	Change current atom from periodic
		table
	Click on atom	Replace atom with current atom
	Build: Fragment	Choose fragment for insertion
View (Rotate)	Drag	Rotate X,Y
	Shift-drag	Rotate Z
View (Translate)	Drag	Translate X,Y
View (Zoom)	Drag up	Bigger
	Drag down	Smaller
Adjust	Click on background	Select entire molecule
	Click on atom	Select first atom
	Shift-click on atom	Select another atom
	Select 2 atoms, Adjust: Bond	Change bond length
	Length	
	Select 3 atoms; Adjust: Bond Angle	Change bond angle
	Select 4 atoms; Adjust: Dihedral	Change dihedral angle
	Angle	
	Ctrl-click on atom	Change atom hybridization
	Ctrl-click on bond	Change bond order

Common WebMO Editor Actions

A significant amount of chemistry is built into the WebMO Editor. When creating a molecule, only backbone atoms need to be entered. WebMO can then automatically add all hydrogen atoms and make reasonable approximations for all bond lengths and angles. The precise dihedral conformation of the molecule can then be adjusted, if desired.

The WebMO Editor allows one to work with groups of atoms, by inserting pre-defined fragments and by manipulating selected portions of the molecule.

WebMO Pro offers a Z-Matrix Editor, which allows one to edit the Z-matrix that defines the molecular geometry. This advanced feature is useful for defining the molecular coordinate system and for defining coordinates that will be scanned when computing potential energy surfaces.

When the molecule has been created as desired, close the WebMO Editor with File: Close on the menu, the close window control on the Editor window frame, or the Close Editor button on the Build Molecule page. The molecule is then transferred from the WebMO Editor onto the Build Molecule page, from which one can run a computational job with the newly created molecule.

C. Build Tool

The build tool is used to add new atoms, bonds or fragments to a molecule.

Once the WebMO Editor is opened, the build tool is invoked with **Tools**: Build, or by clicking

The WebMO Editor status line indicates the current atom, which is initially carbon. The status line also indicates what operations are permitted at the current time.

To add an atom, simply click in the editor window. To add a bond and atom, click on an existing atom and drag to a new location.

To add a bond between two existing atoms, click on one atom and drag to another atom. To make a multiple bond, drag between the two atoms multiple times. This will cycle the bond order from single to double, triple, and back to single.

To change the default atom, choose Build: H, Build: O, Build: N, or Build: Other... (E). Choosing Build: Other... opens the Periodic Table dialog box, from which one may click on a new atom. The new current atom is reflected on the status line, and subsequent clicks will insert the new atom.

To change the identity of an existing atom, click on the atom. It will change to the new default atom.

If an error is made while building a molecule, use Edit: Undo () and Edit: Redo () to undo and redo editing changes. By default, 5 undo levels are saved, although this can be changed in File: Preferences... (). To delete an atom, choose the adjust tool with Tools: Adjust (), select the atom by clicking on it, choose Adjust: Delete Selection, and return to the build tool with Tools: Build (). One can entirely delete the molecule and start over with File: New.





Peri	odic	Ta	ble														×
Н		Symbol:								C He							
Li	Be	Atomic Number:						6 B C					Ν	0	F	Ne	
Na	Mg											Al	Si	Ρ	S	CI	Ar
Κ	Ca	Sc	Ti	۷	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Υ	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	SЬ	Te	Т	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	lr	Pt	Au	Hg	Ti	ΡЬ	Bi	Po	At	Rn
Fr	Ra	Ac															
				Ce Th	Pr Pa	Nd U	Pm	Sm	Eu	Gd	Тb	Dy	Ho	Er	Tm Canc	Чb	Lu
Warr	ning:	Арр	let V	/indo	WV									_			

Periodic Table Dialog Box

One does not need to add hydrogen atoms or worry about precise bond lengths and angles when building a molecule. The cleanup tool (\square) may be used at anytime to add hydrogen atoms and idealize all bond lengths and angles.

It may be useful to the rotate (a), translate (b), or zoom (a) the structure when building a molecule. Choosing any of these controls activates the view tool, after which the build tool (a) must be chosen again to continue adding to the structure.

D. View Tool

The view tool is used to adjust the view of the molecule in 3-D space. The molecule may be rotated, translated, or zoomed. The view tool is used to inspect and orient the molecule as it is being built.

Once the WebMO Editor is opened, the view tool is invoked with Tools: View, or by clicking \square , \square , or \square on the toolbar. There are three modes in which the view tool operates:

- Rotate
- Translate

• Zoom

To activate a particular mode, choose View: Rotate (\square), View: Translate (\square), or View: Zoom (\square).

The WebMO Editor status line indicates which view mode is active, as well as how to manipulate the molecule in the current mode.

In rotate mode, dragging the mouse rotates the molecule about the x and y axes (in the plane of the screen), and control-drag rotates the molecule about the z axis (perpendicular to the screen). In translate mode, dragging the mouse translates the molecule in the xy plane (plane of the screen). In zoom mode, dragging up makes the molecule bigger, and dragging down makes the molecule smaller.

If the molecule is moved or zoomed out of the editor field-of-view, i.e., if the molecule is "lost," choosing Edit: Find will translate the molecule back to the center of the editor window, re-rient the molecule, set the zoom factor appropriately, and set the rotation origin to the center of the molecule.



E. Adjust Tool

The adjust tool is used to define the precise conformation (bond length, bond angle, and dihedral angle) of atoms in the molecule. It is used to adjust the order of bonds and hybridization of atoms. Also, as described in a subsequent section, it is used to manipulate a selected set of atoms relative to the rest of the molecule.

Once the WebMO Editor is opened, the adjust tool is invoked with **Tools:** Adjust, or by clicking **I** on the toolbar.

The WebMO Editor status line states that the adjust tool is active and indicates how to select atoms. Once atoms are selected, the status line displays the corresponding bond length, bond angle, or dihedral angle.



Definitions of Bond Length, Bond Angle, and Dihedral Angle

The adjust tool acts on selected atoms. To select multiple atoms, click the first atom and shiftclick all subsequent atoms. (More precisely, clicking an atom defines it as the selection set, and shift-clicking an atom toggles it in or out of the selection set.) To select the entire molecule (or more precisely, all atoms and bonds in the Editor), click anywhere in the background.

The order in which atoms are selected is extremely important. Bond and dihedral angles depend on the order of selected atoms. Also, when changing the geometry of a molecule, **the first selected atom is the atom that is moved**.

When 2, 3, or 4 atoms are selected, the current value of the corresponding bond length, bond angle, or dihedral angle is displayed in the status line. To change the bond length, bond angle, or dihedral angle, choose Adjust: Bond Length (, Adjust: Bond Angle (), or Adjust: Dihedral Angle (), respectively. Enter the new desired value into the dialog box, optionally click Apply preview the change, and click OK to make the change.

Note that **the first selected atom is the atom that is moved** when making geometry adjustments. Also, all atoms attached to the first atom will move, unless they form part of a ring system. Bond lengths are displayed in Angstroms, and bond angles are displayed in degrees. When changing a bond angle, all bond lengths remain unchanged. When changing a dihedral angle, all bond lengths and angles remain unchanged.



Adjust Tool and Dihedral Angle Dialog Box

To adjust the order of a bond, ctrl-click the bond to bring up a bond order context menu, from which the desired bond order (single, double, triple) may be chosen. To adjust the hybridization of an atom, ctrl-click the atom to bring up a hybridization context menu, from which the desired hybridization (sp, sp2, sp3, dsp3, d2sp3) may be chosen.



Bond Order and Atom Hybridization Context Menus

F. Cleaning-Up Structures

Cleaning-up a chemical structure adds missing hydrogen atoms and sets bond lengths and angles to ideal values. The resulting structure is usually a good guess of the starting geometry for a calculation, although one may need to manually adjust dihedral angles to achieve a specifically desired conformation.

The clean-up procedure involves three steps using basic organic chemistry rules:

- Add Hydrogens: Empty valencies are filled with hydrogen atoms
- Hybridization: Each atom is assigned a hybridization

• Geometry: Bond lengths and angles are set to ideal values

These steps should be carried out in order, since each step relies on the previous step having already been completed.

To invoke all three clean-up steps with a single command, choose Clean-Up: Comprehensive (1).



Before and After Comprehensive Clean-Up

The rules used for cleaning-up structures are based on stable organic molecules. If one is building a transition state or radical, it is often necessary to manually adjust the molecule during the clean-up process. Thus, one might build the molecular backbone, choose Clean-Up: Add Hydrogens, manually add or delete some hydrogen atoms, choose Clean-Up: Hybridization, manually adjust the hybridization if an atom, and finally choose Clean-Up: Geometry.

To clean up just a portion of the molecule, select the atoms to be cleaned-up, choose Clean-Up: Selection Only, and then choose the clean-up action that is desired. Atoms that were not selected will not be affected.

G. Fragments and Fragment Library

Pre-defined structure fragments can be inserted into the editor, saving the effort of manually creating them and adjusting their geometry.

To insert a fragment, choose the build tool and choose Build: Fragment.... Select the desired category and fragment, and click OK. Click in the editor to add the chosen fragment.

Choose Fragment	×
Category:	Functional Groups 💌
Fragment:	Phenyl 💌
OK	Cancel
Warning: Applet Window	

Fragment Library Dialog Box

When adding a fragment to an existing molecule, it is often useful to move the fragment relative to the molecule. Choose the adjust tool, and select the fragment by dragging a box around it or by selecting an atom and choosing Adjust: Select Molecule. Then use the Adjust: Rotate Selection and Adjust: Translate Selection menu items.

The fragment library can be extended by the WebMO system administrator using the Fragment Manager. Any WebMO job can be imported into the fragment library, making the molecular structure readily available within the editor.

H. Working With Selections

It is often useful to manipulate a subset of the atoms in the editor, e.g., a portion of a molecule or a separated fragment.

To create a selection set, one must first invoke the adjust tool with Tools: Adjust (L). Several methods exist for creating a selection set:

- Click on the first atom and then shift-click on subsequent atoms
- Drag a box around a group of atoms and bonds
- Click on a single atom and choose Adjust: Select Molecule to select all connected atoms

To clean-up a selection, choose Clean-Up: Selection Only, and then choose the clean-up action that is desired (Add Hydrogens, Hybridization, Geometry, or Comprehensive). Atoms that were not selected will not be affected.

To move a selection relative to the rest of the atoms in the editor, use the Adjust: Rotate Selection and Adjust: Translate Selection menu items. When rotating a selection, dragging the mouse rotates the selection about the x and y axes (in the plane of the screen), and control-drag rotates the selection about the z axis (perpendicular to the screen). When translating a selection, dragging the mouse translates the molecule in the xy plane (plane of the screen), and control-drag translates the selection along the z axis (perpendicular to the screen). Atoms that were not selected are not moved.

To duplicate a selection, choose Adjust: Duplicate Selection and then click to insert a copy of the selection. The copied fragment can be moved relative to the molecule by invoking the adjust

tool, selecting the fragment, and choosing Adjust: Rotate Selection or Adjust: Translate Selection.

To find a selection, choose Adjust: Find Selection. The zoom factor is adjusted, and the selection is centered and oriented in the editor. In addition, the center of the selected atoms becomes the rotation origin when the Adjust: Rotate Selection or View: Rotate are used.

To delete a selection, choose Adjust: Delete Selection which deletes the selected atoms and bonds from the molecule.



Moving a Selection Relative to Other Atoms in the Editor

I. Z-Matrix Editor (Pro)

WebMO automatically creates a z-matrix (geometry defined by bond lengths, angles, and dihedral angles) to specify the geometry and coordinates of the molecule in the editor. It is sometimes necessary to edit the default z-matrix to specify a particular coordinate for use in a calculation. WebMO Pro provides a Z-Matrix Editor that allows complete control over the z-matrix for the current molecule.

To use the Z-Matrix Editor, choose Tools: Z-Matrix..., which brings up the Z-Matrix Editor dialog box. The atoms in the molecule are listed by element and atom number under the Atom column. The z-matrix entry for each atom is defined by the bond length, angle, and dihedral angle with respect to previously defined atoms under the Na/Length, Nb/Angle, and Nc/Dihedral columns. The molecule in the editor displays the atom number on each atom, so that the entries in the Z-Matrix Editor can easily be visualized.

Z-Matrix	Editor										×
Order	Atom	Na	Length	Opt	Nb	Angle	Opt	Nc	Dihedral	Opt	
1	C1										
2	C2	1	1.499	0 -							
3	C3	2	1.499	0 -	1	59.949	0 -				
4	H4	3	1.095	0 🗸	2	119.973	0 🗸	1	109.469	0 -	
5	H5	1	1.095	0 💌	2	119.961	0 -	3	109.535	0 🗸	
6	H6	1	1.095	0 💽	2	119.980	0 -	3	-109.552	0 💽	
7	H7	2	1.095	0 💽	1	120.013	0 🔹	3	109.475	0 💽	-
8	H8	2	1.095	0 💌	1	119.996	0 -	3	-109.459	0 🔹	F.
		Sta	art		Stop		# Steps				
Scan											
Re	eOrder		ReConne	ect	Opt	All	Fic	k All		ОК	
Warning: /	Applet W	indow									

Z-Matrix Editor Dialog Box

Two steps are required to change the z-matrix for the current molecule: first reorder the atoms as desired, and second adjust the connectivity definitions. These steps must be done in this order.

To reorder the atoms, change the numbering in the **Order** column (negative and decimals are OK) and click the **ReOrder** button. The atoms will be resorted in numerical order. Note that the connectivity definition will likely change during this process.

To adjust the connectivity definitions, change the atom numbers in column Na (Length), Nb (Angle), and Nc (Dihedral) as desired, and click the ReConnect button. Note that atoms can only reference atoms above them in the z-matrix.

The Z-Matrix Editor is used to specify which coordinates should be optimized or fixed during the calculation. To optimize or fix a coordinate, set the corresponding Opt entry to O (optimize) or F (fix), respectively. The Opt All and Fix All buttons optimize and fix all of the coordinates, respectively.

The Z-Matrix Editor is also used to specify that a coordinate should be scanned in the calculation. To scan a coordinate, set the corresponding Opt entry to S (Scan). Then enter the desired Start, Stop, and # Steps values. Note that # Steps represents the number of points *in addition to* the first point.

If an atom is added or deleted, a new default z-matrix is created, and previous z-matrix edits are discarded.

J. Preferences

Visual preferences of the editor can be set with the Preferences dialog box, which is called with File: Preferences... or by clicking the preferences button (E) on the toolbar.

The Atom Size and Bond Size with which atoms and bonds are drawn may customized.

The Background Color of the editor may be specified. White is useful when copying the editor window to the Windows clipboard with Alt-Print Screen and pasting the bitmap image into other applications.

Atom labels may be omitted, displayed as a Symbol, or displayed as the atom Index.

The default number of Undo levels may be reset, or the undo mechanism may be disabled on slower computers.

Preferences	X						
Atom Size(%):	30						
Bond Size(%):	100						
Background color:	gray 💌						
Display:	⊙ None ⊂ Symbol ⊂ Index						
Disable Undo (for slower computers)							
Undo levels:	5						
OK	Cancel						
Warning: Applet Window							

Preferences Dialog Box

K. Help

Choosing Help: Index opens up the Editor Help page for the WebMO Editor in a new web browser window.

The Editor Help page offers brief descriptions of each WebMO Editor menu item. It also has online tutorials for the WebMO Editor, as well as descriptions of the view, build, adjust tools.

The Editor Help page also has links to the Program Help and Administrative Help pages.

3. Running Jobs

A. Overview

After a molecule is built and appears on the Build Molecule page, the next step is to choose the computational engine to carry out the desired job. WebMO supports the following computational chemistry programs:

- Gamess
- Gaussian
- MOPAC

These programs are not part of WebMO and must be installed separately by the system administrator (see http://www.webmo.net/support for instructions).

If more than one computational engine or server is installed, the desired engine and server must be specified. From the Build Molecule page, click Choose Engine to display the Choose Computational Engine page. Select the desired computational chemistry program. WebMO Pro supports multiple computational servers. If a particular server is desired, select the server; otherwise, leave the server at First Available so that it will run as soon as possible. Finally, click Job Options.

If only one computational engine is installed on only one server, then there is no choice of computational engine. From the Build Molecule page, simply click Job Options.

Engine	Description
C Gamess	Ab initio and semi-emperical calculations
Gaussian	Ab initio and semi-empirical calculations
C Mopac	Semi-empirical calculations
Select Server	www.webmo.net

Choose Computational Engine Page

Each computational engine has its own Configure Job Options page (see subsequent sections). The Configure Job Options page permits entry of:

- Job Name
- Calculation type
- Level of Theory

- Basis Set
- Charge
- Multiplicity

There is also an Advanced Options page, on which less frequently used options can be specified.

The different Calculation types are described in the next section. The Job Options and Advanced Options pages for each computational engine are described in subsequent sections.

The Configure Job Options page has a **Preview Input File** box that can be checked. If this option is selected, the input file that will be sent to the computational chemistry program is displayed in an edit box, where it can be viewed and optionally edited.

Clicking Submit Job sends the job to the WebMO job queue, where it is run in turn at the first available opportunity.

Preview Gaussian Input File	
#N HF/3-21G OPT	1
Formyl Fluoride 0 1 C 0 1 B1 F 1 B2 2 A1 H 1 B3 2 A2 3 D1 A1 120.00000 A1 120.00000 D1 150.00000	
D1 1.2750000 B1 1.2750000 B2 1.4900000 B3 1.0900000 B3 1.0900000 B3 1.0900000	

Preview Input File Page

B. Calculation Types

Molecular Energy

A Molecular Energy calculation computes the energy and electronic properties (dipole moment, partial charges, bond orders) of the current atomic configuration using the specified theory and basis set.

Geometry Optimization

A Geometry Optimization calculation finds the nearest energy minimum by minimizing the energy. The resulting energy, electronic properties (dipole moment, partial charges, bond orders), and new geometry are reported. The optimized geometry is the nearest local minimum, which is not necessarily the global minimum.

Transition State Optimization

A Transition State Optimization calculation finds the nearest stationary point by minimizing the gradient. A transition state is a minimum in all normal mode coordinates except one, for which it is a maximum. Locating a transition state can be very difficult, as it is easy to fall into a nearby minimum or other topological feature. To locate a transition states, it is very important to have a very good starting point, perhaps determined by symmetry or by a saddle calculation.

After a transition state calculation has completed, the transition state should be verified by carrying out the following additional calculations:

- A vibrational frequencies calculation which has a single negative (imaginary) frequency
- Forward and reverse IRC calculations which lead to products and reactants

Vibrational Frequencies and Thermochemistry

A Vibrational Frequencies or Thermochemistry calculation finds the normal vibrational frequencies, intensities, and modes of a molecule. The vibrational normal modes and the infrared spectrum may be visualized from the job results page. The vibrational information can be used with the molecular geometry to report thermodynamic quantities (enthalpy, heat capacity, entropy) at a given temperature and pressure (standard conditions by default).

Before carrying out a vibrational frequency calculation, either a geometry optimization or transition state optimization must be carried out so that the geometry is a stationary point, i.e., the gradient is zero. If using MOPAC, the additional keyword PRECISE is recommended when optimizing to insure tight convergence.

A vibrational frequency calculation can be used to characterize a stationary point. All positive frequencies indicates a minimum, one negative (imaginary) frequency indicates a transition state, and more than one negative frequency indicates a "hilltop" or higher-order transition state.

UV-Vis Spectrum

A UV-Vis Spectrum calculation computes excited electronic states, vertical transition energies, and transition intensities. The UV-Vis spectrum may be visualized from the job results page.
Coordinate Scan (Pro)

A Coordinate Scan calculation steps an internal coordinate (bond length, bond angle, or dihedral angle) and computes the energy at each point. The remaining coordinates can be all optimized (relaxed scan), all fixed (rigid scan), or a combination of both.

The Z-Matrix Editor is used to define the coordinate to be scanned (S), and whether the remaining coordinates should be optimized (O) or fixed (F).

The resulting energy values can be visualized or exported in spreadsheet format.

IRC Calculation

An IRC (Intrinsic Reaction Coordinate) Calculation changes the molecular geometry by moving along a normal vibrational mode coordinate, in either the forward or reverse direction. IRC calculations are useful for checking transition state calculations, in order to verify that the reaction coordinate vibrational motion leads to reactants in one direction and products in the other direction.

Saddle Calculation

A Saddle Calculation is a useful way to locate a transition state. Two geometries on opposite sides of the transition state are specified, and the saddle calculation merges the structures together while moving up in energy toward the transition state. The job number of a previously calculated second geometry is specified on the Advanced Options page.

It is essential that both molecular geometries have the same atomic numbering in a saddle calculation. Thus, to generate a second geometry on the other side of the transition state, one must start with New Job Using This Geometry and then edit bond lengths and angles appropriately, taking care not to add or delete atoms which would automatically renumber the atoms.

The result of a saddle calculation should be a geometry that is close to the transition state connecting the two initial geometries. However, a transition state optimization calculation must still be carried out on the result to locate the actual transition state, and the resulting transition state should be verified as discussed above.

Molecular Orbitals (Pro)

A Molecular Orbitals calculation computes the molecular orbitals of the current molecule. From the molecular orbitals, the electron density, electrostatic potential, and frontier orbital densities can be computed. These can all be visualized using the MOViewer helper application, which must first be installed on the client computer.

3. Running Jobs

NMR

A NMR calculation computes the absolute NMR shifts of each atom in the molecule. The NMR shifts of H and C relative to TMS are also provided for the default basis sets. Proton and carbon NMR spectra can be visualized from the job results page.

High Accuracy Methods

A High Accuracy Method is a compound method, such as G2, which results in energy calculations that are accurate to within several kcal/mol for most molecules.

Other

A user specified calculation type may be specified, e.g., "CBS" for the Complete Basis Set compound method in Gaussian. Keywords for other calculations can be found in the documentation that comes with each computational engine. When specifying a calculation type, it is recommended that Preview Input File be checked, so that the input file can be verified and optionally edited.

C. Gamess

Gamess (General Atomic and Molecular Electronic Structure System) is a general ab initio quantum chemistry package that is freely available from the Gordon research group at Iowa State University (http://www.msg.ameslab.gov/GAMESS/GAMESS.html).

The Job Options and Advanced Options pages for Gamess are described below.

C	onfigure G	amess Jol	o Option	S
	Job Name		_	
	Calculation	Molecular Energy	_	
	Theory	RHF -		
	Basis Set	Basic: 3-21G		
	Charge	0		
	Multiplicity	Singlet 💌		
	Preview Input File			
	Advanced Option	ns		

Configure Gamess Job Options Page

Entry	Choices
Job Name	arbitrary name describing the calculation
Calculation	Molecular Energy
	Geometry Optimization
	Vibrational Frequencies
	Transition State Optimization
	IRC Calculation
	Molecular Orbitals
	Other
Theory	RHF
	UHF
	GVF
	Other
Basis Set	Minimal: STO-3G
	Basic: 3-21G
	Routine: 6-31G(d)
	Accurate: $6-311+G(d,p)$
	MNDO
	AM1
	PM3
	Other
Charge	, -2, -1, 0, 1, 2,
Multiplicity	Singlet,, Sextet
Preview Input File	view and optionally edit input file

Configure Gamess Job Options Choices

Advanced	d Gamess Job Options - Microse	oft Internet Explorer	_02
Ad	lvanced Gam	ess Job Op	tions
	Symmetry Group	C1 💽	
	Order of n-fold axis	1	
	Solvent	None	
	Cartesian Coordinates		
	CPU %	100	
	Additional Keywords		
	Close		
		initiation and a state	
Done		🚽 🚽 Inte	met

Advanced Gamess Options Page

The symmetry of the molecule may be specified with Symmetry Group and Order of n-fold axis. A Solvent may be specified, although this significantly increases the calculation time. The default specification of molecular geometry is with a z-matrix; however, Cartesian Coordinates

3. Running Jobs

may be used instead. Note that Gamess carries out calculations in Cartesian coordinates by default, regardless of the coordinates used to specify the molecular geometry. CPU% specifies what fraction of the CPU this job should consume. Specifying 100% claims exclusive use of the computational server, whereas specifying 50% would permit another 50% job to run simultaneously on the same server. Additional Keywords permits the specification of additional keywords on the control card. If several keywords are specified, one should preview the input file to insure that line lengths do not exceed the 80 character fortran card limit, inserting a line break if necessary.

D. Gaussian

Gaussian is an electronic structure program that is commercially available from Gaussian, Inc. (http://www.gaussian.com).

The Job Options and Advanced Options pages for Gaussian are described below.

			s opno	
	Job Name			
	Calculation	Molecular Energy		
	Theory	Hartree-Fock 💌		
	Basis Set	Basic: 3-21G	•	
	Charge	0	_	
	Multiplicity	Singlet		
	Preview Input File	e F		
	Advanced Opti	ions		
Tob Manager	Build Molecule	Choose Engine	Job Options	Submit Job

Configure Gaussian Job Options Page

Entry	Choices
Job Name	arbitrary name describing the calculation
Calculation	Molecular Energy
	Geometry Optimization
	Vibrational Frequencies
	Optimize + Vib Freq
	UV-Vis Spectrum
	NMR
	Coordinate Scan
	Bond Orders
	Molecular Orbitals
	Transition State Optimization
	Saddle Calculation
	IRC Calculation (Forward)
	IRC Calculation (Reverse)
	G2 High Accuracy Calculation
	Other
Theory	Hartree-Fock
	B3LYP
	Moller Plesset 2
	Moller Plesset 4
	AM1
	PM3
	UFF Mechanics
	Other
Basis Set	Minimal: STO-3G
	Basic: 3-21G
	Routine: 6-31G(d)
	Accurate: $6-311+G(d,p)$
	Other
Charge	, -2, -1, 0, 1, 2,
Multiplicity	Singlet,, Sextet
Preview Input File	view and optionally edit input file

Configure Gaussian Job Options Choices

3. Running Jobs

Output Mode	Normal 💌
olvent	None 💌
xcited State	
lse Checkpoint File	None 💌
ave Checkpoint File	
econd Geometry (job number)	[
lartesian Coordinates	
isable Symmetry	
PU%	100
Idditional Keywords	

Advanced Gaussian Options Page

The level of raw output may be specified as Terse, Normal, or Verbose. A Solvent may be specified, although this significantly increases the calculation time. The input geometry may be read from an existing Checkpoint File, and/or a checkpoint file for the calculation may be created. For a Saddle Calculation, the Second Geometry must be specified by supplying its job number. The default specification of molecular geometry is with a z-matrix; however, Cartesian Coordinates may be used instead. Note that Gaussian carries out calculations with Internal Redundant Coordinates by default, regardless of the coordinates used to specify the molecular geometry. One can Disable Symmetry, which is necessary if the symmetry of the molecule changes during the calculation. CPU% specifies what fraction of the CPU this job should consume. Specifying 100% claims exclusive use of the computational server, whereas specifying 50% would permit another 50% job to run simultaneously on the same server. Additional Keywords permits the specification of additional keywords in the route card.

E. Mopac

Mopac (Moleculat Orbital PACkage) is a general-purpose semiempirical quantum mechanics program. Versions 7 and earlier are public domain and are freely available from a variety of sources (http://www.ccl.net, http://www.webmo.net, and others), and versions 2000 and later are commercially available from the CAChe Group of Fujitsu, Inc. (http://www.cachesoftware.com).

The Job Options and Advanced Options pages for Mopac are described below.

Configure Mopac Job Optio Eile Edit View Favorites	ns - Microsoft Internet Exp Iools <u>H</u> elp	lorer			
	Configure N	1opac Job	Options	8	Ľ
	Job Name		_		
	Calculation	Molecular Energy	•		
	Theory	PM3			
	Charge	0			
	Multiplicity	Singlet 💌			
	Preview Input File				
	Advanced Optic	ons			
Job Manager	Build Molecule	<u>Choose Engine</u>	Job Options	Submit Job	
					7
Done				Internet	10

Configure Mopac Job Options Page

Entry	Choices
Job Name	arbitrary name describing the calculation
Calculation	Molecular Energy
	Geometry Optimization
	Vibrational Frequencies
	Thermochemistry
	Transition State Optimization
	Saddle Calculation
	IRC Calculation (Forward)
	IRC Calculation (Reverse)
	Coordinate Scan
	Molecular Orbitals
	Other
Theory	PM3
	AM1
	MINDO/3
	Other
Charge	, -2, -1, 0, 1, 2,
Multiplicity	Singlet,, Sextet
Preview Input File	view and optionally edit input file

Configure Mopac Job Options Choices

3. Running Jobs



Advanced Mopac Options Page

The Symmetry Number of the molecule may be specified for thermochemistry calculations. A Solvent may be specified, although this significantly increases the calculation time. For a Saddle Calculation, the Second Geometry must be specified by supplying its job number. The default specification of molecular geometry is with a z-matrix; however, Cartesian Coordinates may be used instead. Mopac carries out the calculation in the coordinates that are used to specify the molecular geometry. A filename of External Parameters may be supplied. CPU% specifies what fraction of the CPU this job should consume. Specifying 100% claims exclusive use of the computational server, whereas specifying 50% would permit another 50% job to run simultaneously on the same server. Additional Keywords permits the specification of additional keywords in the keyword section. Some useful additional keywords are

PRECISE - Tighten convergence criteria MMOK - Add a mechanics correction to amide linkages GEO-OK - Allow atoms to be closer than 0.8 Angstom

F. Failed Calculations

When running computational chemistry jobs, especially on new molecular systems, it is inevitable that some jobs will fail. After diagnosing the cause of failure, changes can be made that allow most jobs to run successfully.

The most important step in analyzing a failed job is to view the output file by clicking Raw Output in the Job Manager. The cause of failure will usually be indicated near the end of the file. Once the cause of failure is identified, appropriate corrective action can be taken.

Some common causes of job failure (and possible solutions) include:

- A job exceeding the maximum job time limit (use a lower theory or smaller basis set)
- Incorrect specification of charge or multiplicity (specify correctly)
- Change of molecular symmetry during the calculation (choose Disable Symmetry from the Advanced Options)

- Problem with geometry specification (choose Cartesian Coordinates from the Advanced Options, redefine the z-matrix, or specify GEO-OK in Mopac)
- Optimization failed to converge (Restart the job or start from a different initial geometry)

If a job has failed, it is possible to restart the job from the last valid geometry, which could be either the initial geometry or the last step of a geometry optimization, by clicking **Restart** in the Job Manager.

A. Molecular Geometry

After the Job Manager indicates that a job has successfully completed, clicking the corresponding View button (View) will display the job results in graphical and tabular form.

At the top of the job results page is the job number, title, calculation type, and computational engine.

The final molecular geometry is shown in a 3-D display. The molecule can be rotated (\square), translated (\square), and zoomed (\square) by clicking the appropriate toolbar button and dragging the mouse as described in the WebMO Editor section. Clicking select (\square) on the toolbar and then selecting 2, 3, or 4 atoms will display the corresponding bond length, bond angle, or dihedral angle in the status line. Clicking preferences (\blacksquare) on the toolbar allows the atom size, bond size, background color, and atom label to be customized.



3-D Display of Molecular Geometry

Below the 3-D display are buttons to accomplish the following tasks:

- Job Manager: Return to the Job Manager
- New Job Using This Geometry: Go to the Build Molecule page and display the current molecule
- Raw Output: View the output file produced by the computational engine

- Reset Viewer: Return the molecule to its default viewpoint and configuration
- Export Molecule: Export the displayed molecule in a variety of formats
- Output Files: View and download all input and output files (Pro)

B. Calculated Quantities

The quantities that are calculated are specific to the calculation type and computational engine. Information that can be displayed in tabular form includes:

- Symmetry
- Energy (HF, MP2, MP4, CCSD, CBS-4, G2, Heat of Formation, etc.)
- Thermodynamic Quantities (enthalpy, heat capacity, entropy, etc.)
- Rotational Constants
- Dipole Moment
- Partial Charges
- Bond Orders
- Vibrational Mode Symmetries and Frequencies
- Molecular Orbital Symmetries and Frequencies
- NMR Absolute and Relative Shifts

Some quantities (partial charges, bond orders, NMR shifts) are listed with respect to atom numbers, which are shown in the 3-D molecular display.

alculated Q	uantiti	les						
Quantity	Value							
Route	PM3 BC	NDS CH	ARGE=0	SINGLET				
Symmetry	CS							
Heat of Formation	-88.7986	63 kcal/m	ol					
Dipole Moment	2.449 E	lebye 🔵	View					
Partial Charges					ĩ			
	Atom	Symbol	Charge	View				
	1	С	.3518					
	2	0	3096					
	3	F	1497					
	4	Н	.1075					
Bond Order	Atom	Sy	mbol	С	0	F	Н	
	1	С		3.463329				
	2	0		1.941851	10.527764			
	3	F		.958313	.119915	13.195342		
	4	Н		.932955	.029636	.025849	.796528	
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Calculated Quantities

C. Dipole Moment and Partial Charges

In addition to being listed as numerical values, some quantities may be displayed visually. Clicking the View button corresponding to Dipole Moment or Partial Charges will display the quantity in the 3-D display.



3-D Display of Dipole Moment and Partial Charges

The dipole moment vector is centered at the center of mass and its length is set such that 1 Debye corresponds to 1 Angstrom. When viewing partial charge, the radius of each atom is proportional to its partial charge, and negative atoms are colored red while positive atoms are colored blue. This color code is consistent with the MOViewer convention of small \leftrightarrow large values being mapped onto red \leftrightarrow blue colors.

Clicking Reset Viewer will return the 3-D display to its default view of the molecular geometry.

D. Normal Modes

A Vibrational Frequencies or Thermochemistry calculation displays the vibrational frequencies of the normal modes in tabular form.



Table of Vibrational Frequencies

Individual normal modes can be displayed in the 3-D display by clicking the View button associated with each mode. The magnitude of the normal displacement vectors is controlled by the Normal Mode Amplitude value. A negative Normal Mode Amplitude reverses the directions of the arrows.



C-H Stretching Normal Mode

The entire infrared spectrum can be displayed by clicking the IR Spectrum View button. Computed peak positions and intensities are used, and the peak width is controlled by the Peak Width value.

E. NMR, UV-Vis, and Infrared Spectra

In addition to peak position listed in tabular form, computed spectra are available after performing their corresponding calculations.

Spectrum	Calculation
NMR	NMR
Infrared	Vibrational Frequencies
	Thermochemistry
UV-Vis	UV-Vis Spectrum

Computed Spectra Calculations

Computed spectra are displayed by clicking the spectrum View button. Peak positions and intensities are based on computed values. The peak widths for the spectra are controlled by the Peak Width value on the job results page.





13C and 1H NMR Spectra



Infrared Spectrum



UV-Vis Spectrum

Spectra can be customized in the Spectrum Viewer window. To zoom into a defined region, click the Zoom in button and then define a zoom box by dragging. To zoom out, click the Zoom out button and then click on the spectrum. To return to the default zoom, click the Reset Zoom button. The Options button offers control over the line color, line type, range of the plot, and axis labels. To close the Spectrum Viewer window, click the Close button.

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Range	Axes		Upper Right:	-8.0	23.0		y-axis:	-5.0	25.0	5.0
OK	Revert	Cancel	OK	Cancel			OK	Cancel	(
Warning: Applet Windo	w		Warning: Apple	t Window		Warning: Applet Window				

Spectrum Viewer Options Dialog Boxes

F. Coordinate Scans (Pro)

Coordinate scans are produced by defining the internal coordinate to be scanned using the Z-Matrix Editor and then performing a Coordinate Scan calculation.

Coordinate scans can be displayed by clicking the View button, or the data can be converted into spreadsheet format and downloaded locally by clicking the **Download** button.

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	90.0000	5.55077	
	94.0000	3.04720	
	98.0000	.97778	
	102.0000	64609	
	106.0000	-1.83206	
	110.0000	-2.60413	
	114.0000	-2.99537	
	118.0000	-3.04857	
	122.0000	-2.81062	
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View Coordinate Scan

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3	94	3.0472							
4	98	0.97778							
5	102	-0.64609							
6	106	-1.83206							
7	110	-2.60413							
8	114	-2.99537							
9	118	-3.04857							
10	122	-2.81062							
11	126	-2.32992							
12	130	-1.65651							
13	134	-0.83932							
14	138	0.07364							
15	142	1.03897							
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Download Coordinate Scan

G. MOViewer (Pro)

Molecular orbitals and their dependent functions may be viewed with the MOViewer helper application, which is compatible with Microsoft Windows (and Linux under WINE). Because of the intensive calculations required to compute and render 3-D surfaces are intensive, MOViewer is a client application that must be installed on each client computer. To install MOViewer on a computer, perform any Molecular Orbitals calculation, e.g., a Hartree-Fock STO-3G Molecular Orbitals calculation on H₂O. View the job results, scroll to the bottom of the Molecular Orbitals output, and click the 'Help Viewing MOs' link. On the WebMO MO Viewing Help page, click the 'MOViewer Setup program' link, and save the InstallMOViewer.exe program to the client computer's hard disk. Run the InstallMOViewer program and follow the prompts to install the MOViewer program.

A Molecular Orbitals calculation displays the symmetry, occupancy, and energy of each molecular orbital. There are also View buttons to view each molecular orbital, the electron density, electrostatic potential, and frontier densities.



Table of Molecular Orbitals

Clicking the View button corresponding to a molecular orbital will transfer the orbital to the client computer. The selected molecular orbital isosurface is displayed around the molecule. Occupied orbitals are displayed in red/blue by default, and unoccupied orbitals are displayed in yellow/green. Several orbitals can be displayed in separate windows for comparison.

When prompted to save the resulting .MO file, **Internet Explorer users** should choose to "Open this file from its current location" to open the file in MOViewer and then click Open to open the file in MOViewer. To automatically open orbitals in MOViewer, unselect the "Always ask before opening this type of file" option at the bottom of the dialog. This will cause .MO files to be opened automatically without further prompts.

The first time **Netscape users** attempt to view an orbital, Netscape will return an "Unknown file type" prompt. Select "Pick App..." and browse to and select the MOViewer executable (MOViewer.exe) located by default in C:\Program Files\MOViewer. When prompted to save the resulting .MO file, choose "Open it" and then click Open to open the file in MOViewer. To automatically open orbitals in MOViewer, unselect the "Always ask before opening this type of file" option at the bottom of the dialog. This will cause .MO files to be opened automatically without further prompts.



Occupied and Unoccupied Molecular Orbitals

Electron density is computed from the sum of squares of occupied molecular orbitals. Displaying an Electron Density isosurface represents the size of a molecule.

Various quantities, such as the Electrostatic Potential and Frontier Densities, can be "painted" on the electron density isosurface. In all cases, smaller values are represented by red, and larger values are represented by blue. Thus, red represents negative regions and blue represents positive regions on an electrostatic potential surface. For example, the electrostatic potential surface of water, H_2O , is red (negative) around the oxygen and blue (positive) around the hydrogens.



Electron Density and Electrostatic Potential Surfaces

Frontier density surfaces are computed from the magnitudes of molecular orbitals available for attack by an electrophile, nucleophile, or radical. The result is a "bull's eye" pattern with blue representing the largest probability of attack. For example, the electrophilic (HOMO) frontier density surface of formaldyhde, H_2CO , is blue (maximum value) around the oxygen. The surface indicates that protonation will occur at the oxygen in the molecular plane. The nucleophilic (LUMO) frontier density surface of formaldyhde is blue (maximum value) around carbon. The surface indicates that nucleophilic attack will occur at the carbon out of the molecular plane.



Electrophilic (HOMO) and Nucleophilic (LUMO) Frontier Density Surfaces

Surface	Color	Interpretation
Molecular Orbital	Red/Blue	occupied orbital
	Green/Yellow	unoccupied orbital
Electron Density	Gray	isosurface
Electrostatic Potential	Red	negative region
	Blue	positive region
Electrophilic (HOMO)	Blue	region most susceptible to
Frontier Surface		attack by an electrophile
Nucleophilic (LUMO)	Blue	region most susceptible to
Frontier Surface		attack by a nucleophile
Radical Frontier	Blue	region most susceptible to
Surface		attack by a radical

Color Interpretation of Surfaces

The appearance of each surface can be customized with the Edit: Preferences... dialog box. Increasing the number of Grid Points smooths the displayed surface, but increases the calculation time. The Iso Values MO and ED define the isosurface value for the molecular orbitals and electron density, respectively. Padding adds additional distance around the molecule during the isosurface calculation, so that larger orbitals can be viewed without "holes" in them from the edge of the grid volume. Decreasing the Opacity of the surface allows the molecule to be viewed within the displayed surface. Although smooth isosurfaces are displayed by default, checking Wireframe displays see-through wireframe surfaces. Unchecking Display Isosurface removes the isosurface from the display so that only the molecule is visible.

The appearance of the molecule can be controlled by varying the Atom Size. Checking Display Axes will display the cartesian axes, so that orbitals can be more easily identified. The Colors of the Background, Occupied Orbital, and Unoccupied Orbital can be customized.

Continuous varying quantities, e.g., electrostatic potentials and frontier densities, are painted on the specified electron density isosurface so that color represents the value of the quantity. When Auto Scale Range is checked, **the color map automatically ranges from red representing the smallest displayed value to blue representing the largest displayed value**. The numeric values corresponding to red and blue can be specified with Mapped Values (Min/Max), if desired, for example to compare different chemical compounds using the same color map.

Clicking the Apply or OK button applies the changes to the active window. Checking Apply to All Open Windows on OK applies the changes to all windows, so that they are consistent and can be compared.

Preferences	×
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Opacity	100%
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🔽 Display Isosurface	
Molecule Properties	
Atom Size	30%
Display Molecule	
🗖 Display Axes	
Colors	
Background	
Occupied Orbital	
Unoccupied Orbital	
Mapped Values (Min/	Max) 0
🔽 Auto Scale Range	,
Apply to All Open 1	Windows on OK
🔲 Save as Default	
OK Cance	Apply Defaults

MOViewer Preferences Dialog Box

H. Export Molecule

The final molecular geometry of a calculation can be exported in a variety of formats: MOL, PDB, XYZ, Gaussian, and Mopac. On the job results page, click the Export Molecule button below the 3-D molecule display. Choose the desired format and click the Export Molecule button to display a text representation of the molecule. Either copy and paste the text into another application, or save the webpage to a file. If you have configured a program, e.g., chime

(http://www.mdlchime.com) or rasmol, to view .mol, .pdb, or .xyz files, checking Open in External Viewer will cause the molecule to be automatically opened in the chosen program.



Export Molecule Dialog Box



Exported Molecule as Text and into External Viewer

I. Spreadsheet Summary (Pro)

Job results can be exported into a spreadsheet by selecting the jobs and clicking the **Spreadsheet** button on the Job Manager page. Open the resulting file from its current location, or save it to disk if desired. The selected jobs are listed in rows and the calculated quantities are listed in columns on the resulting spreadsheet, making it straightforward to create tables of results and to compare jobs.

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	Number	Name	Description	Date	Status	Time	Actions
•	23	H2CO	Geometry Optimization - Gaussian	11/15/2002 15:04	Complete	20.4 sec	View
•	24	H2CO	Geometry Optimization - Gaussian	11/15/2002 15:04	Complete	21.4 sec	View
V	25	H2CO	Geometry Optimization - Gaussian	11/15/2002 15:04	Complete	28.5 sec	View
•	26	H2CO	Geometry Optimization - Gaussian	11/15/2002 15:05	Complete	46 sec	View
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Selecting Multiple Jobs for Spreadsheet Display

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1	Job Nurr	nber,	Job Nar	ne	Job Descr	iption	Basis	HF Er	ergy		Dipole	Moment	CPU	l time	
2		23	H2CO		Geometry	Optimization	STO-3G	-112.3	54346879	Hartree	1.5370	Debye	20.4	sec	
3		24	H2CO		Geometry	Optimization	3-21G	-113.2	21820005	Hartree	2.6584	Debye	21.4	sec	
4		25	H2CO		Geometry	Optimization	6-31G(d)	-113.8	66331244	Hartree	2.6659	Debye	28.5	sec	
5		26	H2CO		Geometry	Optimization	6-311+G(d,p)	-113.9	02801805	Hartree	2.8148	Debye	46 s	ес	
6															
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Spreadsheet Display of WebMO Jobs

J. Output Files (Pro)

Every file related to a job can be individually viewed or downloaded using the Output Files button on the job results page.

Click the Output Files button on the job results page to display a directory listing of all input and output files for the job. Choose whether you wish to view the file as text or download the file as binary, and then click the filename.

The Output Files feature permits inspection of the actual input and output files used for a particular job. It also permits output files to be downloaded and viewed with separate post-processing and visualization programs, such as Molekel (http://www.cscs.ch/molekel) or Molden (http://www.cmbi.kun.nl/~schaft/molden.html).

Filename	Туре	Size	Timestamp
input.xyz	• Text C Binary	161 bytes	11/15/2002 15:05
connections	• Text • Binary	58 bytes	11/15/2002 15:05
<u>zmatrix</u>	• Text • Binary	53 bytes	11/15/2002 15:05
input.com	• Text C Binary	154 bytes	11/15/2002 15:05
<u>summary</u>	• Text • Binary	179 bytes	11/15/2002 15:05
pid	• Text • Binary	5 bytes	11/15/2002 15:06
output.log	• Text C Binary	43437 bytes	11/15/2002 15:07
output properties	• Text • Binary	446 bytes	11/15/2002 15:07
output.xyz	• Text C Binary	120 bytes	11/15/2002 15:07

Output Files Listing

5. Job and Profile Management

A. Job Manager

The central tool for managing submitted and completed computational chemistry jobs is the Job Manager.

The top of the Job Manager displays account information (username, total time limit, job time limit) and the current number of queued jobs. The main portion of the Job Manager is a list of completed and submitted jobs, which can be managed with various actions. Buttons at the bottom of the Job Manager allow one to create new jobs, import existing jobs, and edit one's profile, and access online help.

Jobs are initiated by clicking the **Create New Job** button at the bottom of Job Manager. After a job has been submitted it will appear the Available Jobs list with the status of Queued or Running. After the job completes, the status will be changed to Complete or Failed. The status of the job list can be updated with the **Refresh** button.

IMPORTANT TIP: Set your web browser to load documents every time, rather than pulling them from its cache. **Internet Explorer** users should click **Tools**, click **Internet Options**..., click the **General** tab, and click the **Settings**... button under "Temporary Internet files." Select "Every visit to the page" under "Check for newer versions of stored pages." **Netscape** users should click View, click Options..., click the + sign next to Advanced, and click Cache. Select "Every time" under "Document in cache is compared to document on network."

Actions that may be carried out on listed jobs are:

- Filter: Display only jobs meeting selected filter conditions
- Kill: Kill a queued or running job
- Raw Output: Monitor a running job, or view a failed job
- View: View a completed job
- Restart: Restart a failed job by placing last valid geometry on Build Molecule page

Previous chapters describe:

- Create New Job: Bring up Build Molecule page with the WebMO Editor
- Spreadsheet: Compare results from multiple jobs

Subsequent sections of this chapter describe:

- Delete: Move jobs to the trash folder
- Download: Transfer jobs from WebMO to your local computer
- Rename: Rename the selected job
- Folders and Move To: Organize jobs into user-defined folders (Pro)

5. Job and Profile Management

- Import Job: Transfer jobs from your local computer to WebMO
- Edit Profile: Change your user preferences

Other buttons on the Job Manager are:

- Refresh: Update the list of jobs
- About WebMO: Display version information
- Help: Display online help
- Logout: Logout of WebMO

Total Time Limit 4:38:03 Job Time Limit 10:00 Jobs Queued 0							
a	ilable	Jobs - Inb	OX Show all	Show all	Show all		Filter
	Number	Name	Description	Date	Status	Time	Actions
1	15	phenol	Optimize + Vib Freq - Gaussian	11/13/2002 13:43	Complete	1:40	View
1	16	para-quinone	Geometry Optimization - Gamess	11/15/2002 13:46	Complete	2:36	View
1	17	acetamide cation	Geometry Optimization - Gaussian	11/15/2002 13:52	Failed	0.9 sec	Raw Output Restart
1	18	acetamide	Geometry Optimization - Gaussian	11/15/2002 13:57	Complete	3:07	View
1	19	formyl fluoride	Geometry Optimization - Mopac	11/15/2002 13:57	Complete	0 sec	View
1	Select A	u .					
De	lete D	ownload Rer	name Spreadsheet		Folders M	ove To	-Move to Selected Folder- 💌

WebMO Job Manager

B. Folders (Pro)

WebMO Pro allows users to organize their jobs by creating folders for storing completed jobs. WebMO users have only Inbox and Trash folders. WebMO Pro users can create an unlimited number of user-defined folders, which is ideal for organizing multiple projects or saving important jobs without cluttering up the Inbox. **To create a new folder**, click the **Folders** button at the bottom of the Job Manager job listing. Enter a **Folder name** and click the **Create** button. A green "Folder successfully created" message is displayed confirming that the new folder has been created. Either create additional folders or click the **Return to Job Manager** button.

To rename a folder, select an existing folder as the Target folder, specify a new name as the New Folder, and click the Rename button. To delete a folder, select an existing folder as the Target folder and click the Delete button. Jobs in the deleted folder are moved to the Inbox.

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Folder Management

To display the jobs in a different folder, select the desired folder in the -Move to Selected Folder- dropdown box and click the Move To button. The Job Manager now displays jobs in the new folder.

To move completed jobs to another folder, check the checkboxes corresponding to the jobs, select the desired folder in the -Move to Selected Folder- dropdown box, and click the Move To button. The selected jobs are moved to the selected folder, and the selected folder is displayed.

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Moving a Job to a New Folder

Submitting a new job automatically changes the current folder to the Inbox, where are running and completed jobs are initially placed.

5. Job and Profile Management

Deleted jobs are moved from the current folder to the Trash folder, but not actually deleted from the file system. To permanently delete a job from the file system, display the Trash folder and delete the jobs again.

C. Download

Completed jobs may be downloaded from the WebMO server to the user's local machine. This is useful for backing up individual jobs, archiving jobs prior to their deletion from the WebMO server, or transferring jobs from one WebMO implementation to another.

Downloaded jobs are in tar file format and include the entire directory of the completed job. This allows the user to examine the raw input and output files, as well as all additional information saved or parsed by WebMO. This also permits importing of the downloaded archive back into WebMO with no loss of information.

To download completed jobs, check the checkboxes corresponding to the jobs and click the Download button. Save the file to the desired location when prompted.

The resulting file can be examined with tar, WinZip, or other programs able to extract files from a tar archive.

D. Import

Existing output files can be imported into WebMO. This is useful for importing previously computed jobs into the WebMO environment, using WebMO's visualization capabilities for jobs calculated elsewhere, transferring jobs between WebMO implementations, or importing previously downloaded WebMO jobs back into WebMO.

To import existing output files or downloaded WebMO archives, click the Import button at the bottom of the Job Manager job listing. For an existing output file, enter a Job Name, select the File Type, specify the location of the output file on the remote (server) computer or on the local computer, and click the Import Job button. For a previously downloaded WebMO archive, specify the location of the local file and click the Import Job button. The specified jobs are imported and appear in the Inbox folder.

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Import an Existing Job	AAA
Job Name	
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Choose one of the following three options:	
l) Remote output file	
2) Local output file	Browse
3) Local WebMO archive	Browse
Import Job Return to Job Manager	664
Done	Sector Se

Importing an Output File or WebMO Archive

E. Rename

To rename a job, check the corresponding checkbox and click the Rename button. The new name can be entered into the pop-up dialog box.

Renamed jobs appear with their new names in the WebMO environment. However, the raw output file, which contains the original job name as a job title, remains unchanged.



Renaming a Job

F. Delete

To delete jobs displayed in the Job Manager, check the corresponding checkboxes and click the **Delete** button.

Deleted jobs are simply moved to the Trash folder, rather than permanently deleted from the server file system. They can be undeleted by displaying the Trash folder and moving the jobs into another folder.

To permanently delete jobs from the server file system, display the Trash folder by selecting the Trash folder and clicking the Move To button. Check the checkboxes corresponding to the jobs to be permanently deleted, and click the Delete button. Confirm that the selected jobs will be permanently deleted by clicking the OK button.

Jobs that are permanently deleted cannot be restored. However, if they were previously downloaded to the local computer, they can be imported back into WebMO.

G. Edit Profile

To change user settings, click the Edit Profile button in the Job Manager. Users may change their password. Users may also specify their email address and choose to receive email notification of completed jobs.

Users may also choose to display job results in a new window, rather than replacing the Job Manager window, by checking View job in new window. This is useful when it takes a long time to regenerate a lengthy job list when returning to Job Manager after viewing a job. When this option is checked, one can simply close the job results page and use the existing Job Manager window.

To enact changes, click the Submit button. A confirmation message will be displayed. When finished making changes, scroll down to the bottom of the page and click the Return to Job Manager button.



Edit User Profile

6. WebMO Administration

A. Overview

After the initial installation, all WebMO configuration and administration is done through a web browser interface. To access the WebMO administration webpages, login as the user "admin" with the admin password.

The WebMO administrator can:

- Add, edit, disable, or delete WebMO users
- Limit total or job CPU time for WebMO users
- Kill running or queued jobs from all WebMO users
- View, download, or delete completed jobs from all WebMO users
- Configure WebMO settings
- Check for WebMO updates
- Add to the WebMO fragment library
- Configure remote computational servers
- Configure computational chemistry program settings



Login as admin to Access WebMO Administration Pages

6. WebMO Administration

B. User Manager

To add, edit, disable, or delete users, click the User Manager link on the WebMO Administration page. An alphabetized list of WebMO users is displayed.

To add a new user, click the **New User** button. On the New User page, specify a username and password, and confirm the password. Optionally provide an email address. If appropriate, specify total and job time limits. Click the **Submit** button. A confirmation message is displayed.

The Total time limit entry specifies the total amount of time that the user has remaining in the users' account. After a job completes, the job time is subtracted from the total. When the total time limit reaches zero, the user may not run any more jobs until the WebMO administrator adds more time. The Job time limit entry specifies the maximum time that a job may run, after which it is automatically killed by WebMO. To specify no time limit, enter "N/A" or "-1".

To edit an existing user, click the Edit button. The WebMO administrator may change the user password, email address and notification status, and time limits. Click the appropriate Submit button for the changes to take effect.

To disable or enable users, click the corresponding Disable or Enable button. Disabled users are not permitted to login to WebMO, although their jobs are available in the administrator Job Manager. To delete a user, click the Delete button. A dialog box asks whether to permanently delete the files of the deleted user from the server file system.

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Username	Status	Actions			1	
admin	Enabled	Edit				
iohnson	Disabled	Edit	Enable	Delete		
volik	Enabled	Edt	Disable	Delete		
schmidt	Enabled	EdR	Disable	Delete		
smith	Enabled	Edit	Disable	Delete		

User Manager and Edit User Profile

Password		
Confirm password		
E-mail	smith@webmo.net	
E-mail	smith@webmo.net	
E-mail notification	-	
view job in new window	15664	
rmie mint (s)	15004	

C. Job Manager

The Job Manager allows the administrator to monitor all queued and running jobs and to view, download, and delete any completed job.

The administrator Job Manager is very similar to a user's Job Manager. The primary differences are:

- The administrator job manager displays the jobs of all users
- The administrator job manager does not display jobs in folders
- Although completed jobs can be viewed, new jobs cannot be created and run from the admin account

To kill a running or queued job, click the corresponding Kill button. To update the Job Manager display, click the Refresh button at the bottom of the page.

To download completed jobs, check the corresponding job checkboxes and click the **Download** button. Similarly, to view a spreadsheet summary of completed jobs, check the corresponding job checkboxes and click the **Spreadsheet** button (Pro).

To delete jobs, check the corresponding job checkboxes and click the **Delete** button. A confirmation screen warns that the jobs will be permanently deleted. Note that unlike a user's Job Manager, jobs are not first moved into a Trash folder. Instead, the administrator Job Manager immediately deletes jobs from the file system.

Because the administrator job manager typically displays many jobs, filters are available to view jobs by computational engine, user, date, and status. Choose the desired filter conditions, and click the Filter button to reduce the number of displayed jobs.

When viewing jobs as admin, it is useful to have checked View job in new window in the admin user profile, available by editing the admin user in User Manager. This saves the time of regenerating a lengthy job listing when returning to Job Manager after viewing a job. Simply close the separate job results window, rather than click the Return to Job Manager button.

6. WebMO Administration

/ebMO Job Manager							
		Show all 💌	Show all 💌	Show all 💌	Show all 💌		Filter
Number Name	Description Usern	Username	ame Date	Status	Time	Actions	
3	methane	Geometry Optimization - Gaussian	polik	5/6/2002 1:13	Complete	14.6 Бөс	View
4	Methane	Vibrational Frequencies - Gaussian	polik	5/6/2002 2:41	Complete	8.9 Бес	View
5	phenol	Optimize + Vib Freq - Gaussian	smith	5/14/2002 0:20	Complete	1:53	View
6	para-quinone	Geometry Optimization - Gamess	smith	5/14/2002 0:23	Complete	2:37	View
7	acetamide cation	Geometry Optimization - Gaussian	smith	5/14/2002 1:42	Failed	l sec	Cutout

Administrator Job Manager

D. System Manager

The WebMO daemon and WebMO preferences are controlled by the System Manager.

The status of the WebMO daemon is displayed as either "Not running" or "Running". Note that the WebMO daemon only runs when jobs are queued and/or running. When there are no queued or running jobs, the WebMO daemon does not run. Under normal conditions, the daemon status should not be changed. If the daemon is stopped, then all currently running jobs are killed! Starting a daemon with no queued jobs has no effect, as the daemon automatically exits when the job queue is empty.

The queue status is normally enabled. Disabling the queue allows currently running jobs to complete, but does not start any queued jobs. This capability is useful if the computer needs to be taken down for maintenance while jobs are still queued. After the computer is brought back up, the queue should be enabled and the WebMO daemon should be manually started, so that queued jobs are run.

WebMO preferences may be specified in the System Manager. The Server name is an arbitrary descriptive string for the WebMO computational server. The Registered user is an arbitrary string displayed on the WebMO Login page. The Background graphic is the filename for the background image on all WebMO pages, and the Table background is the color for all tables displayed by WebMO.

The System scratch directory is the location where WebMO stores all scratch files created by computational engines. This should be a location with a large amount of free space that is writable by all computer users, e.g., /tmp or /scratch.

Click the Submit button to implement preference changes.

vebiviO Syst	tem Manager	
Daemon status: <mark>Not runni</mark>	ng Stat	
Queue status: Enabled	Disable	
Server Name	www.webmo.net	
Registered user	Computational Chemistry on the WWW	
Background graphic	background_dna.gif	
Fable background	#99cccc	
	Itmp	

System Manager

E. Version Manager

The version, license number, and total jobs run are displayed by the Version Manager.

The Version Manager also checks whether the most recent version of WebMO is running and informs you if an update is available. A link is provided to the WebMO download area for obtaining updates.

When updating WebMO, the location of the globals.int configuration file must be specified. The Version Manager displays the location of this file, which can then be input into the upgrade script.



Version Manager

F. Fragment Manager

The Fragment Library permits users to insert fragments when building molecules with the WebMO Editor.

The WebMO administrator can add fragments to the Fragment Library with the Fragment Manager. The source of the fragment must be an existing WebMO job. To add a fragment, specify the Job number from which to import the fragment geometry, specify a Category for the fragment, e.g., rings, and specify a Fragment name, e.g., benzene. Click the Submit button, and the fragment will be added to the Fragment Library.

Fragments are stored in the {cgiBase}/interfaces/fragments.txt file.



Fragment Manager

G. Remote Server Manager (Pro)

WebMO Pro supports multiple computational servers accessible from a single webserver. This permits a single instance of WebMO to run jobs on any available computational server. There are significant advantages of using one copy of WebMO Pro over using several copies of WebMO on multiple computers. WebMO Pro automatically runs the submitted job on the first available server, without having to manually check the job status on each server. Also, WebMO Pro saves all of a user's jobs in one location, rather being spread out over multiple computers.

The requirements for configuring a remote computational server are:

- Existing account: The administrator must have an existing account on the remote server. It is preferable that this account be dedicated to WebMO.
- rsh/rcp or ssh/scp: The WebMO webserver account must be able to access the remote compserver account with rsh/rcp or with ssh/scp. It is essential that the webserver account be able to execute commands in the compserver account without being prompted for a password. For example,
\$ rsh -l webmo compserver.domain.edu ls should list the files on the remote computational server, where webmo is the account under which the webserver cgi scripts run.

Detailed **instructions for configuring a remote computational server** may be found by clicking the Help button on the Remote Server Manager. Briefly, insure that the above pre-requisites are met, and test that the webserver can execute remote commands on the compserver. Add the remote server to WebMO in the Remote Server Manager by specifying the requested information, clicking the Submit button, and waiting 5 to 60 seconds for a confirmation message. Then, enable the computational engine interfaces for the remote server in the Interface Manager by selecting the remote server, clicking the Change button, and clicking the Enable button for each available interface. Finally, configure each new interface in the *{Computational Engine}* Manger by selecting the remote server, clicking the Change button, editing the preferences such as the path to the executable, and clicking the Submit button.

Exiting remote servers can be upgraded, renamed, or deleted from the Edit Existing Remote Server section of the Remote Server Manager.

Remote servers should be upgraded whenever WebMO itself is upgraded. **To upgrade a remote server**, specify the remote Target Server, and click the **Upgrade** button. Waiting 5 to 60 seconds for a confirmation message. In effect, the upgrade process deletes and adds the remote server, with the end result that the latest WebMO scripts are copied to the remote server.

To rename a remote server, choose the remote Target server, specify a new Server name, and click the **Rename** button. **To delete a remote server**, choose the remote Target server, specify a new Server name, and click the **Delete** button.

6. WebMO Administration

webMornemote Servi]le <u>E</u> dit ⊻iew F <u>a</u> vi	r Manager - Microsoft Intelnet Explorer rites Iools Help	
VebMO]	Remote Server Manag	er
	g	
Add New Rei	note Server	
Server Name	Remote 1	
Hostname	server.domain.edu	
Username	webmo	
Home Directory	/home/webmo	
Scratch Directory	/mp	
Protocol	rsh 💌	
Add Help Ret	um to Admin	
Cdit Existing	Remote Server	
Target Server	elect Server to Edit-	
Server Name		
Server riante		
Update Rename	Delete Help Return to Admin	

Remote Server Manager

H. Interface Manager

The Interface Manager enables and disables the computational engines supported by WebMO.

Since WebMO Pro supports multiple computational servers, if the desired server is not displayed at the top of the page, it must first be selected selecting the remote server and clicking the **Change** button.

The current status of each interface is displayed as either Disabled or Enabled. Click the Enable or Disable button to change the availability of the computational engine on the specified server. When a computational engine is enabled, a corresponding *{Computational Engine}* Manger will appear on the main administration menu.



Interface Manager

I. Computational Engine Managers

Computational Engines are configured with the corresponding {Computational Engine} Manger.

Since WebMO Pro supports multiple computational servers, if the desired server is not displayed at the top of the page, it must first be selected selecting the remote server and clicking the **Change** button.

The *{Computational Engine}* Manger varies with each computational chemistry program. In general, one specifies the version of the program, the location of the executable, and other directory locations.

If present, the Suggest button may be used to fill in some entries. Specify the program directory, click the Suggest button, and as much information as possible will be automatically filled in.

The minimum, maximum, and default CPU percentage can be specified. CPU% specifies what fraction of the available CPU on the server that this engine may consume. Specifying 100% claims exclusive use of the computational server, whereas specifying 50% would permit another 50% job to run simultaneously on the same server. CPU intensive programs are typically set to run at 100% for a single CPU server, or at 50% for a dual CPU server. Less demanding programs may be set at lower percentages so that several instances may run simultaneously on the same CPU. For example, setting Gaussian to 70% and Mopac to 30% would allow 1 instance of Gaussian; 1 instance of Gaussian and 1 instance of Mopac; or 1, 2, or 3 instances of Mopac to run simultaneously. Users are able to change the CPU% between the minimum and maximum CPU percentage specified on this page.

Once the computational program is configured, click the Submit button for the settings to take effect. A green confirmation message, or a red error message, will be displayed.

6. WebMO Administration

		Eile Edit ⊻iew Favo	rites Iools Help
		WebMO (Gaussian Manager
🖉 WebMO Gamess Manag	er - Microsoft Internet Explorer	Server - www	v.webmo.net
<u>File E</u> dit <u>V</u> iew F <u>a</u> vori	tes Iools Help	- Server	-Solort Sover to Edit.
WebMO (Gamess Manager	Gaussian version	
Server - www.	webmo.net	Gaussian root directory	/usr/local
Server	-Select Server to Edit-	Executable	/usr/local/g98s/bsd:/usr/local/g98/bsd:/usr/local/g98s/private
Gamess version	25 MAR 2000	Archive directory	/usr/local/q98/arch
Gamess directory	/usr/local/gamess	Main directory	/usr/local/a98s/bsd:/usr/local/a98/bsd:/usr/local/a98s/private
Gamess binary	gamess.00.x	Library directory	/usr/local/a98s/bsd./usr/local/a98/bsd./usr/local/a98s/private
(name, not path) Ddikick binary		Basis directory	/usr/local/q98s/basis/usr/local/q98/basis
(name, not path)	ddikick×	CPU %	Min 0 Max 100 Default 100
Note: The suggest but given the Gamess dire to succeed.	ton will attempt to fill as much information as possible netory. This information is required if the suggest function is information is required if the suggest function is	given the Gaussian of function is to succeed the Gaussian root dir	vot directory. This information is required if the suggest l. For example, if Gaussian is installed in /usr/local/g94 ectory would be /usr/local. Internet
WebMO Mopae Manage Ele Edt View Favor WebMO N Server - www.	er Microsoft Internet Explorer		
Server	-Select Server to Edit-		
Mopac version	Mopac 7		
Mopac path	/usr/local/mopac7/mopac.exe		
External parameter			
CPU %	Min 0 Max 100 Default 100		
Submit Help F	Return to Admin	_	
Done	🖉 Internet		

Gamess, Gaussian, and Mopac Managers

J. Customization

Look and Feel

Aspects of WebMO's look and feel may be customized with the System Manager, which is accessible from the admin account. The Registered user is an arbitrary string displayed on the WebMO Login page. The Background graphic is the filename for the background image on all WebMO pages. The Table background is the color for all tables displayed by WebMO.

The name of the WebMO computational server displayed on the Choose Computational Engine page is specified as the Server name in the System Manager. The name of each remote computational servers is specified as the Server name in the Remote Server Manager.

It is possible to edit the *.html files in the {htmlBase} directory of a WebMO installation, so long as only the displayed text is changed, i.e., form and javascript variables may not be changed.. However, beware that support cannot offered when files are directly edited, and edited files will not survive the version upgrade process.

Calculation Templates

Each calculation type for a computational engine is defined by a job template file, e.g., gaussian.tmpl, which is located in the $\{cgiBase\}/interfaces$ directory. Additional jobs may be defined by adding to this template file. The syntax of job template files is described in online documentation that may be accessed from any Help button. Scroll down to the bottom of the help page, click on the 'Program' link, and then click on the 'Creating job templates' link.

Changes to template files in the WebMO {cgiBase}/interfaces directory affect all users. However, WebMO Pro also permits users to define their own private templates by inserting a job template file into their own WebMO directory, {userBase}/{username}. These calculation types will appear only on that user's Configure Job Options page.

Beware that global template files in the *{cgiBase}/interfaces* directory are overwritten with new files in the version upgrade process. However, previous global template files are automatically backed up by the upgrade, so that additional or customized calculation types can then be manually copied to the upgraded template files.

Basis Set Choices

In order to not overwhelm the novice computational chemistry user, WebMO provides only a limit range of basis set choices for each computational engine on the Configure Job Options page. Advanced users may wish to extend this list to include their favorite basis sets.

In the file {*htmlBase*}/{*engine*}.html, there is a SELECT NAME="basisSet" section. Add additional OPTON statements to this section following the format used for the other basis sets. The new basis sets will then be available to all users.

Beware that changes to the global basis set choices in the *{htmlBase}/{engine}*.html file will not survive the version upgrade process, as these files are overwritten with new files. Thus, customized file should be backed up, so that the additional basis sets can be manually copied to the upgraded template files.

A. WebMO Editor

1. Creating Structures Using WebMO

Use the WebMO Editor to build the following molecules.

A. Propene, $CH_3CH=CH_2$

B. Aspirin, C₉H₈O₄

Use the Fragment Library (Build: Fragment...) in the WebMO Editor to create the following molecules. When working with two fragments, it is often useful to select one fragment, and then rotate or translate just the selected fragment with Adjust: Rotate Selection or Adjust: Translate Selection. It is also useful to cleanup just a portion of the molecule by selecting the atoms for cleanup, choosing Clean-Up: Selection Only, and then choosing Clean-Up Comprehensive.

OH

0

0



From the WebMO Build Molecule page, import the following molecules as chime structures. Locate these structures by performing an internet search for the terms "chime" and "molecule", where "molecule" is the molecule of interest. When viewing these molecules as chime structures in a web browser, save them to you local hard disk by right-clicking and choosing File: Save Molecule as... in either MOL or PDB format. On the WebMO Build Molecule page, click the

Import Molecule button. On the Import Molecule page, choose the proper format, browse to the saved file, and click the Import Molecule button

- E. Taxol, C₄₇H₅₁NO₁₄
- F. Buckminsterfullerene, C₆₀

USEFUL TIP: In Windows, Alt-Print Scrn copies the active window to the clipboard as a bitmap graphic image. This is very useful for inserting WebMO images into other applications, such as Microsoft Word or PowerPoint. It is often preferable to change the WebMO Editor background color from gray to white with File: Preferences.... Also, the resulting image usually needs to be cropped. This can be done within Word or PowerPoint from the picture toolbar with the crop tool. Or it can be done by pasting the image into an image-editing program, such as the Paint program. Activate Paint, choose Edit: Paste to paste the image into Paint, use the rectangle to the clipboard (or Edit: Copy to... to save the rectangle to disk), and finally activate Word and paste the rectangle into Word.

B. Input and Output Files

2. Previewing the Input File

Build formaldehyde, H_2CO , using WebMO. Perform a Molecular Energy calculation on it. Check the **Preview Input File** checkbox before submitting the job. Identify the purpose of each part of the input file.

3. Locating Results in the Output File

Build formaldehyde, H_2CO , using WebMO. Perform a Molecular Energy calculation on it. View the results using WebMO. Also view the raw output file by clicking the Raw Output button. Make a table that lists each item on the WebMO results page and the corresponding line(s) in the raw output file. Make a list of items in the raw output file that are not listed on the WebMO results page.

C. Molecular Properties

4. Dipole Moment of Propene

Build propene, CH₃CH=CH₂, using WebMO. Perform a Molecular Energy Hartree-Fock 3-21G calculation on it. Provide an image of the dipole moment of propene. Note that WebMO follows the chemistry convention of the dipole moment pointing from positive to negative, *i.e.*, towards excess electron density. Speculate on the source of the dipole moment in propene.

5. Molecular Orbitals of Formaldehyde (Pro)

Build formaldehyde, H_2CO , using WebMO. Perform a Molecular Orbital Hartree-Fock STO-3G calculation on it.

From the energies, shapes, and composition of the molecular orbitals, classify each molecular orbital as bonding, anti-bonding, non-bonding or core.

Provide images of the HOMO-1, HOMO and LUMO. Describe each of these orbital as sigma or pi and as bonding, anti-bonding, or nonbonding.

Repeat the molecular orbital calculation using the 3-21G basis set. What atomic orbitals are used for row 2 atoms (O and C) in each basis set? For H atoms?

6. ¹³C NMR shifts of butane, butene, and butyne

Build butane, butene, and butyne. Adjust the dihedral angles to result in planar, staggered conformations. Perform a NMR Hartree-Fock 3-21G calculation on each.



butane 2-butene 2-butyne

If any of the jobs failed, view the Raw Output from Job Manager and determine why the job failed. Report the line(s) in the output file that indicates the reason for failure, and explain why this happened. Build the molecule again and re-run the job, but on the Configure Job Options page, click the Advanced Options button and choose Cartesian Coordinates.

Computational chemistry programs compute absolute chemical shifts. WebMO converts these chemical shifts to shifts relative to TMS. Make a table with columns for compound, C atom (outer or inner), absolute shift, relative shift, and literature value. Justify these chemical shifts based on your chemical knowledge.

compound	C _{outer}	C _{inner}
butane	13.4	25.2
trans-2-butene	17.6	126.0
2-butyne	—	73.6

Silverstein, Bassler, and Morril, *Spectroscopic Identification of Organic Compounds*, 5th ed. (Wiley, New York, 1991), Tables 5.2, 5.6, 5.8

D. Geometry Optimizations

7. Conformers of *n*-Butane

Use the WebMO Editor to build *n*-butane, C_4H_{10} . Set the initial C_1 - C_2 - C_3 - C_4 dihedral angle to 30°. Perform a Geometry Optimization calculation on the molecule, and record the optimized dihedral angle and energy. Repeat the calculation with an initial dihedral angle of 150°.

Explain why different structures result from the two optimizations. Characterize each optimized structures as either a local or global minimum.

8. Potential Energy Surface of Methyl Rotation in *n*-Butane (Pro)

Build and clean-up *n*-butane, C_4H_{10} , with an initial dihedral angle of 180°. Open the Z-Matrix Editor with Tools: Z-Matrix... First, verify that the four carbons are listed first and that a terminal carbon atom is the fourth atom (for which a dihedral angle is defined). If this is not the case, reorder the atoms appropriately in Order column and click the ReOrder button. Second, change the Dihedral Opt entry for the terminal carbon from O (= optimize) to S (= scan). Third, define the scan by setting Start to 0, Stop to 180, and # Steps to 18. This will result in 19 calculations as the dihedral angle takes on values of 0, 10, 20, ..., 180. Click OK to close the Z-Matrix Editor.

Perform a Coordinate Scan calculation with PM3 theory. [If using MOPAC, click the Advanced Options button and specify the additional keyword PRECISE.] Preview the input file and note how the scanned coordinate is specified.

After the job is completed, view the results and view the coordinate scan. Indicate where the *trans* and *gauche* conformers on the potential energy surface plot. Explain the difference in the energies of these two conformers.

9. VSEPR Theory

Calculate the energies of planar, tee, and pyramidal ClF₃ by performing Geometry Optimization calculations using Hartree-Fock theory with the STO-3G basis.



To build a particular geometry, construct ClF_5 , set the hybridization of the central Cl atom to dsp3 with the Adjust tool by control-clicking on Cl, choose Clean-Up: Geometry (not Comprehensive!), and finally delete the undesired F atoms.

If a particular geometry optimization calculation fails to converge, click the **Restart** button in Job Manager, and view the last computed geometry. If this conformation is different than the initial geometry, what does this mean about the stability of the initial geometry?

Construct a table with columns for initial geometry and optimized energy. Explain whether or not your results agree with VSEPR (Valence Shell Electron Pair Repulsion) theory learned in General Chemistry.

Optionally, verify that PM3 Geometry Optimizations give a different result.

10. Conformers of Vinyl Alcohol

Build vinyl alcohol-0°, vinyl alcohol-180°, acetaldehyde-0°, and acetaldehyde-60°.



Perform a Geometry Optimization Hartree-Fock 3-21G calculation on each.

If using WebMO Pro, select the four jobs in Job Manager and click the **Spreadsheet** button to obtain an immediate comparison among the four calculations. Otherwise, view the results of each job.

Make a table with columns for molecule, number of optimization steps, energy (Hartree), relative energy (kcal/mol). The relative energy should be calculated relative to the global minimum. 1 Hartree = 627.5095 kcal/mol.

For one of these jobs, report the keywords that control the type of calculation being run. Also report the text from the corresponding output file indicating that the optimization has converged. Discuss the physical meaning of the convergence criteria.

11. Transition State of Vinyl Alcohol

Build an approximate transition state for the isomerization of vinyl alcohol-0° and vinyl alcohol-180° as follows. View a successful geometry optimization of vinyl alcohol, and choose New Job Using This Geometry. Adjust the H-O-C=C dihedral angle to 90°. Perform a Transition State Optimization Hartree-Fock 3-21G calculation.

Make a table with columns for conformation and relative energy (kcal/mol). Include the two stable conformations and the transition state in the table.

Report the keywords for this calculation. Report any text in the output file that indicates a Transition State Optimization differs from a Geometry Optimization.

12. Geometry Optimization of Ammonia and Formamide

Build and optimize the geometry of ammonia, NH₃, and of formamide, H₂NCHO. Insert a picture of each optimized geometry. Explain the difference in planarity using your chemical knowledge.

13. Transition State of Silane Elimination Reaction

In this exercise, the transition state for the reaction $SiH_4 \rightarrow SiH_2 + H_2$ will be found.



Build SiH₄ and perform either a PM3 or a Hartree-Fock 3-21G Geometry Optimization on it. After the calculation has completed, note its job number, and view the job. Choose New Job Using This Geometry. Adjust the geometry of the molecule as follows. Adjust the bond length two Si-H bonds to 3.0 Angstroms. Adjust the H-Si-H bond angle for these two lengthened bonds to 15°. Verify that the distance between these two H atoms is now 0.78, which is similar to the H₂ bond length of 0.74 Angstroms. Perform a Saddle Calculation at the level of theory used for the previous geometry optimization. Before submitting the job, click the Advanced Options button, and enter the job number of the previous optimization for the Second Geometry. [If using MOPAC, specify the additional keyword GEO-OK, which allows the calculation to proceed

despite the short distance between the H atoms.] Close the Advanced Job Options window. Check Preview Input File and submit the job.

Describe the general appearance of the input file. Specifically, how does it differ from other input files? Submit the job.

Provide a picture of the transition state for this reaction. Which H atoms are forming molecular hydrogen? What is their bond length, and how does that compare to the atom distance between the two H atoms in SiH_2 ? in H_2 ? How does their bond angle with Si compare to the SiH_2 bond angle?

Describe how the transition state search algorithm for a saddle calculation differs from a Transition State Optimization. When would you use each algorithm?

E. Frequency Calculations

14. Normal Vibrational Modes of Formaldehyde

Build formaldehyde, H_2CO , and perform a Geometry Optimization PM3 calculation on it. View the result, click on New Job Using This Geometry, and perform a Vibrational Frequencies PM3 calculation. View the result, and view each vibrational mode. Fill in the following table of vibrational frequencies by visually identifying the description of each normal mode.

Mode	Description	PM3 Frequency (cm ⁻¹)	Literature Frequency (cm ⁻¹)
ν_1	sym CH stretch		2811
ν_2	CO stretch		1756
V ₃	CH ₂ bend		1500
ν_4	out-of-plane bend		1170
v ₅	antisym CH stretch		2861
ν_6	CH ₂ rock		1251

15. Stationary Points of Vinyl Amine

Build planar and pyramidal vinyl amine, CH₂=CHNH₂.



For planar vinyl amine, adjust the hybridization of N to sp^2 and then clean up the geometry. Be sure to adjust the dihedral of the amine group appropriately for each molecule. For each conformation, optimize the geometry and calculate vibrational frequencies with a PM3 (or Hartree-Fock 6-31G(d) or better) calculation.

Make a table with columns for conformation, energy, and type of stationary point. Characterize each stationary point as a minimum or transition state using the frequency results.

Provide a picture of the vibrational mode corresponding to the reaction coordinate for inversion about the nitrogen atom.

16. Stretching Frequencies of Carbonyl Groups

Calculate the C=O stretching frequency of formamide, acetaldehyde and acetyl chloride.



Perform Optimize Geometry and Vibrational Frequencies (or Optimize+Vib Freq) Hartree-Fock 3-21G calculations for each molecule. Computed vibrational frequencies are systematically high and are routinely scaled to better match experiment. The scaling factor for Hartree-Fock 3-21G calculations is 0.9085. Make a table with columns for molecule, calculated CO stretch frequency, scaled CO stretch frequency, and experimental frequency (indicated above).

Comment on the absolute and relative accuracy of frequency calculations.

17. Transition State for 1,3 Hydrogen Shift of Fluoropropene

Build the transition state for the 1,3 hydrogen shift of fluoropropene.



Do not do a comprehensive cleanup, as the Add Hydrogens function uses rules that are applicable to stable molecules, not transition states. Instead, manually add the hydrogens, including a hydrogen that is bonded to both C1 and C3. Adjust the hybridization of C2 to sp^2 , and clean up the geometry only. Adjust the H-C2 bond angle appropriately so it is symmetric with respect to the ring. Perform an Optimize Transition State PM3 calculation on the molecule. If the job was successful, view the result to see if the molecule looks as expected. If the job failed, rebuild the transition state but try adjusting the C-C-C bond angle to approximately 100° while maintaining the symmetry of the ring (*i.e.*, increase C1-C2-C3 by 15°, and then increase C3-C2-C1 by 15°).

Create a new job using the optimized transition state geometry. Perform a Vibrational Frequencies PM3 calculation on the previously optimized geometry. View the transition state.

Insert a picture of the nuclear motion at the transition state. How do you know that it is a transition state?

Build and optimize the geometries of the reactant and product for this reaction. Make a table with columns for species and energy, and include the energies of the reactant, transition state, and product. What is the reaction barrier for 1,3 hydrogen shift of fluoropropene in kcal/mol?

18. Thermochemistry of $CH_3CHO \rightarrow CO + CH_4$ in the gas phase

Build and perform Geometry Optimization and Vibrational Frequencies (or Optimize+Vib Freq) Hartree-Fock 6-31G(d) calculations on acetaldehyde, carbon monoxide, and methane. To speed up your calculation, first pre-optimize the acetaldeyhde geometry using PM3 theory or a smaller basis set.

Make a table of calculated values with columns for molecule, Cv, S, E298, H298, and G298.

Visit the NIST webbook (http://webbook.nist.gov/chemistry) and make a table of experimental values with columns for molecule, C_p , S, and $\Delta_f H$ (kcal/mol).

Compute C_p from your calculations for each species by using the relationship that $C_p = C_v + R$ for an ideal gas.

Compute $\Delta_{rxn}H$ from your calculations by appropriately combining H_{298} values and converting to kcal/mol. 1 Hartree = 627.5095 kcal/mol. Compute $\Delta_{rxn}H$ from the experimental data by appropriately combining $\Delta_{f}H$.

Comment on the agreement between calculation and experiment by comparing C_p , S, and $\Delta_{rxn}H$ values in a table.

F. Model Chemistry

19. Basis Set Effects on Hydrogen Fluoride

Perform Geometry Optimization and Vibrational Frequencies (or Optimize+Vib Freq) calculations using MP2 theory for hydrogen fluoride (HF) with the following basis sets: STO-3G, 3-21G, 6-31G(d), and 6-311+G(d,p).

If using WebMO Pro, select the four jobs in Job Manager and click the **Spreadsheet** button to obtain an immediate comparison among the four calculations. Otherwise, view the results of each job.

Make a table with columns for basis set, bond length, dipole moment, vibrational frequency, energy, and CPU time. Also include the experimental values $(0.9171\text{ Å}, 1.91 \text{ D}, \text{ and } 4139 \text{ cm}^{-1})$ in the table.

Comment on the effect of basis set on the calculation.

20. Theoretical Method Effects on Hydrogen Fluoride

Perform Geometry Optimization and Vibrational Frequencies (or Optimize+Vib Freq) calculations with the 6-311+G(d,p) basis set for hydrogen fluoride (HF) using the following methods: HF, MP2, MP4, B3LYP. (Note that you already did the MP2 calculation in the previous problem.)

If using WebMO Pro, select the four jobs in Job Manager and click the **Spreadsheet** button to obtain an immediate comparison among the four calculations. Otherwise, view the results of each job.

Make a table with columns for method, bond length, dipole moment, vibrational frequency, energy, and CPU time. Also include the experimental values $(0.9171\text{ Å}, 1.91 \text{ D}, \text{ and } 4139 \text{ cm}^{-1})$ in the table.

Comment on the effect of theoretical method on the calculation.

21. Compound Method Calculation of Ozone Destruction by Atomic Chlorine

Use Gaussian to perform CBS-4M calculations on atomic Cl (doublet), O_3 (bent geometry, singlet), OCl (doublet), and O_2 (triplet). [It has been observed that OCl must be built with oxygen as the first atom; otherwise, the CBS-4M portion of the calculation fails.] When configuring Gaussian job options, set Calculation = "Other(CBS-4M)", Theory = "Other()", and Basis Set = "Other()".

Make a table with columns for molecule, energy, and enthalpy. Use your results to calculate the enthalpy change of the reaction

$$Cl + O_3 \rightarrow ClO + O_2$$

Compare your results to the experimental value of $\Delta H = -39.1$ kcal/mol.

Is the difference between calculation and experiment in line with what can be expected from compound methods? How does your result compare to Hartree-Fock calculations (such as the previously calculated decomposition of CH_3CHO into CO and CH_4)?

22. CBS-4M Compound Method

The CBS-4M compound method represents a good compromise between computational accuracy and speed.

View the raw output of a CBS-4M calculation for a molecule (not an atom). Copy all the route lines from the output file. Use these lines to explain how the CBS-4M compound method actually works.

G. Partial Charge

23. Partial Charge Analysis of Electrophilic Aromatic Substitution Reactions

The observed isomeric product distribution of electrophilic attack by NO_2^+ on nitrobenzene and chlorobenzene can be analyzed by examining the partial charges on the otho, meta, and para carbons of substituted benzene reactant.



Build nitrobenzene such that the nitro group lies in the molecular plane and has equal NO bond lengths. Pre-optimize this structure with a PM3 calculation. [If using Gaussian, disable symmetry using the Advanced Job Options. The NoSymmetry keyword prevents the job from terminating if the molecular symmetry changes during calculation.] Re-optimize the geometry of nitrobenzene with a Hartree-Fock 3-21G calculation, also disabling symmetry if necessary. The reported partial changes are Mulliken partial charges.

If using Gaussian, use the New Job Using This Geometry button to perform a Single Point calculation at same level of theory with the additional keyword "Pop=NBO". The Pop=NBO or Pop=NPA keywords request that Gaussian perform a Natural Bonding Orbital analysis of the molecule, in which electrons are assigned to "organic chemistry" orbitals as core electron pairs, single bonds, double bonds, lone pairs, etc. Finally, use the New Job Using This Geometry button to perform a Single Point calculation at same level of theory with the additional keyword "Pop=CHelpG". The CHelpG keyword requests that Gaussian calculate an electrostatic potential-derived potential in which atoms are assigned partial charges to match the electrostatic potential at the van derWaals surface. View the Raw Output of each of these jobs and locate the respective partial charges.

Construct a table with columns for isomer (ortho, meta, para), Mulliken partial charge, NBO partial charge, ChelpG partial charge, and observed nitration product distribution percentage. Use these results to explain the preferred site of electrophilic attack by NO_2^+ .

Repeat the above calculations and construct a similar table for chlorobenzene.

Intuitively explain the computed partial charges by drawing resonance structures for nitrobenzene that withdraw π -electron density from the ring and by drawing resonance structures for chlorobenzene that donate π -electron density into the ring.

Comment on the differences among the methods for computing partial charge.

24. Carbocation Intermediate Analysis of Electrophilic Aromatic Substitution Reactions

Aromatic substitution reactions proceed via a carbocation intermediate. The product distribution of an aromatic substitution reaction may be predicted from the relative stabilities of the carbocation intermediates. The aldehyde group is meta-directing for aromatic substitution reactions.



Product	ortho	meta	para
C ₆ H ₄ CHOCl	19%	72%	9%

Build planar benzaldehyde and optimize the geometry with a PM3 calculation. View the partial charges of the ortho, meta, and para carbons (on the side of the ring closest to the H atom of the aldehyde group).

Click New Job Using This Geometry, and open the molecule in the WebMO Editor. Add a chlorine atom to the ortho carbon (on the H atom side of the aldehyde group). Adjust the double bond to the ortho carbon to a single bond. Select the CHCl group, choose Clean-Up: Selection Only, and choose Clean-Up: Comprehensive so that only the new change is cleaned up. Optimize the geometry of this intermediate structure with a PM3 calculation, setting the charge appropriately for a carbocation.

Repeat this to compute the PM3 energies of the meta and para intermediates.

Construct a table with columns for isomer (ortho, meta, para), partial charge, intermediate energy, and observed chlorination percentage. Comment on your results.

H. Potential Energy Surface Scans

25. Rigid Potential Energy Scan of CH Bond Dissociation (Pro)

Build CH_4 and clean up its geometry. Use Tools: Z-Matrix and Fix All coordinates. Scan the C1-H5 bond length from 0.7 to 2.7 in 20 steps. Perform a Hartree-Fock STO-3G Coordinate Scan calculation.

Repeat the coordinate scan with various levels of theory and basis sets, up to a MP2 6-311+G(p,d) calculation.

Download the coordinate scans and use Excel to plot these potential functions in the same figure. Comment on the relative energies of these plots.

Calculate the CH bond dissociation energy in kcal/mol by taking the difference between the minimum and separated energies. Compare your results to an experimental value from a general or organic chemistry textbook. Comment on any discrepancy.

26. Relaxed Potential Energy Scans of NH₃ and H₂O Inversion (Pro)

Build NH_3 with the WebMO Editor. Use Tools: Z-Matrix to scan the H4-N1-H2-H3 dihedral angle from 90 to 270 in 18 steps. Perform a PM3 Coordinate Scan calculation. From the results page, view the Coordinate Scan and determine the barrier height for ammonia inversion in kcal/mol.

Repeat the calculation for H_2O , scanning the H3-O1-H2 bond angle from 90 to 270 in 18 steps. View the Coordinate Scan and determine the barrier for water linearization in kcal/mol. [If using Gaussian, limit the angle scan to 179 degrees, as Gaussian does not permit bond angles to be defined as 180 or greater.]

Speculate on the reason for difference in barrier heights.

Repeat one the above calculations as a rigid scan, holding all variables fixed except for the scanned variable. How does the rigid scan barrier height compare to the previously computed relaxed scan barrier height? Explain the reason for the difference.

I. Bond Orders

27. Bond Orders of Allyl Radical

Build the planar allyl radical C_3H_5 and perform a Geometry Optimization at the Hartree-Fock 3-21G calculation. Note that allyl has an odd number of electrons and is therefore a doublet.



View the output and click New Job Using This Geometry. Run a Gaussian Bond Order calculation at the same level of theory, which performs a NBO (Natural Bonding Orbital) analysis of the Bond Order. Starting with the same same geometry, run a Gamess Molecular Energy UHF (Unrestricted Hartree-Fock) 3-21G calculation of this doublet molecule. Finally, starting with the same geometry, run a Mopac Geometry Optimization job at the PM3 level of theory.

If time permits, run a Gaussian Calculation = "AIM=BondOrders" job at the same level of theory. Be patient since AIM jobs take a relatively long time! View the Raw Output to obtain the AIM bond orders.

Construct a table with columns for NBO, GAMESS, MOPAC, and AIM, and rows for each unique bond order and a row for calculation time. Comment on your table.

J. Isodesmic Reactions

28. Isodesmic Reaction Analysis of CO₂ Heat of Formation

Build and perform Geometry Optimization and Vibrational Frequencies (or Optimize+Vib Freq) calculations on carbon dioxide (CO₂), formaldehyde (H₂CO), and methane (CH₄) at the Hartree-Fock 6-31G(d) level. Tabulate the energy (0 K) and enthalpy (298 K) for each.

Use these results to calculate $\Delta_{rxn}H$ for

 $\rm CO_2$ + $\rm CH_4$ \rightarrow 2 H₂CO

Explain why this reaction is an isodesmic reaction. Explain what kind of computational results can be expected for such reactions.

Combine your $\Delta_{rxn}H$ result with the experimental heats of formation for methane and formaldehyde to predict the heat of formation for carbon dioxide. Compare your predicted heat of formation with the experimental value. Experimental heats of formation may be obtained from the NIST Chemistry Webbook (http://webbook.nist.gov/chemistry).

K. IRC Scans

29. Intrinsic Reaction Coordinate Verification of the $H_2CO \rightarrow H_2 + CO$ Transition State

Compute the H₂CO \rightarrow H₂ + CO transition state by building the following planar structure:



Double check your geometry before proceeding.

Perform a Transition State Optimization Hartree-Fock 3-21G calculation. View the Results, click New Job Using This Geometry, and perform a Vibrational Frequencies job with the same geometry and theory. Report the value of any negative (imaginary) frequencies. Note the energy and H-H bond length.

Using the transition state geometry, perform a Forward IRC calculation with the same theory. View the result and note the energy and H-H bond length. Use this geometry as the starting point for a Geometry Optimization calculation with the same theory. Note the final energy and the H-H bond length.

Again using the transition state geometry, perform a Reverse IRC calculation with the same theory. View the result and note the energy and H-H bond length. Use this geometry as the starting point for a Geometry Optimization calculation with the same theory. Note the final energy and the H-H bond length.

If either Geometry Optimization calculation job fails, view the Raw Output file and determine why the job failed. Report the line(s) in the output file that indicates the reason for failure.

Report all numerical values for energy and H-H bond length in a table. Also, include a sketch of the Potential Energy Surface for the H₂CO \rightarrow H₂ + CO reaction coordinate, along with pictures of the reactant, transition state, and products.

L. Transition States

30. Transition State of Diels-Alder Reaction (Pro)

Addition of cyclopentadiene and acrylonitrile produces the endo norborene product.



Locate the transition state for this reaction by first building the norbornene product. Perform a PM3 geometry optimization of the product, and verify that the resulting geometry is reasonable.

View the result, choose New Job Using This Geometry, and open the molecule in the WebMO Editor. Adjust the two carbon-carbon bond lengths that are formed in the reaction to 2.2 Angstroms, recalling that the first selected atom is the one that is moved. Open the Z-Matrix Editor with Tools:Z-Matrix.... If necessary change the z-matrix connection definition so that the above two carbon-carbon bonds are directly referenced in the z-matrix (in the Na column) and then click the ReConnect button. Fix both bond length to 2.2 by selecting F (fixed) from the corresponding dropdown menu, and click OK. Perform a PM3 Geometry Optimization calculation on this geometrically constrained molecule.

View the result, and verify that the two carbon-carbon bond lengths formed in the reaction are 2.2 Angstroms. Choose New Job Using This Geometry, and perform a PM3 Transition State Optimization calculation.

View the result, note the bond length of the two carbon-carbon bonds being formed, and note the near planarity of the cyclopendiene ring. Choose New Job Using This Geometry, and perform a PM3 vibrational frequencies calculation. Verify that there is a single negative (imaginary) frequency that corresponds to the reaction coordinate. Report the value of the negative frequency and an image of the corresponding vibrational mode.

31. Transition States of Diels-Alder Stereoproducts (Pro)

Substituted reactants undergoing a Diels-Alder reaction can result in various stereoproducts. For example, the addition of acrylonitrile to 5-fluorocyclopentadiene leads to four possible stereoproducts.



Endo products are generally favored over exo products. Anti products are preferred for alkyl substituted cyclopentadiene, and syn products are preferred for alkoxy or halide substituted cyclopentadiene.

The preferred product can be predicted by comparing the energies of the transition states.

Start with the norbornene transition state in the previous exercise. Open the molecule in the WebMO Editor, and make appropriate substitutions for the transition state to a particular product. Select only the changed atoms, choose Clean-Up: Selection Only, and then choose Clean-Up: Comprehensive. Perform a PM3 Transition State Optimization calculation, followed by a Vibrational Frequencies calculation if desired. Repeat for the other stereoproducts.

Make a table with columns for stereo product and energy. Is the lowest energy transition state consistent with the experimentally observed stereoselectivity?

Optionally, repeat the calculations with 5-methylcyclopentadiene. Does the lowest energy transition state change?

32. Transition State of Keto-Enol Tautomerization

Acetaldehyde can isomerize to vinyl alcohol via proton migration.



Locate and verify the transition state for this reaction as follows. Build the above conformer of acetaldehyde, and perform a PM3 Geometry Optimization calculation.

View the results, and choose New Job Using This Geometry. Open the molecule in the WebMO Editor, and edit the bonds to convert the molecule in vinyl alcohol taking care not to delete or add atoms. Add a bond between the migrating methyl proton to the oxygen atom, adjust the CO double bond to a single bond, adust the CC single bond to a double bond, and delete the bond between the migrating methyl proton and the carbon atom. It is critical to not delete or add any atoms so that the same atom ordering and z-matrix definition is used for both molecules. Choose Clean-Up: Hybridization and Clean-Up: Geometry (but not Clean-Up: Comprehensive, which would invoke Add Hydrogens). Perform a PM3 Geometry Optimization calculation of this vinyl alcohol molecule. Note the job number of this vinyl alcohol calculation.

View the results of the optimized acetaldehyde job again, and choose New Job Using This Geometry. Perform a PM3 Saddle Calculation. Before submitting the job, click the Advanced Options button, and enter the job number of optimized vinyl alcohol as the Second Geometry. Close the Advanced Job Options, and submit the job.

View the results of the saddle calculation, choose New Job Using This Geometry. Perform a PM3 Transition State Optimization calculation.

View the results of the transition state optimization job, and choose New Job Using This Geometry. For cosmetic purposes, open the molecule in the WebMO Editor and adjust the bonds in the HOCC 4-membered rings to single bonds. Perform a PM3 Vibrational Frequencies calculation. Verify that there is a single negative (imaginary) frequency, and report its frequency. Verify that the corresponding vibrational mode corresponds to proton migration. What other motions are involved at the transition state?

Optionally, verify that this geometry is a transition state by performing Forward and Reverse IRC calculations, optimizing the resulting geometries, and comparing them to the reactant and product.

M. Excited States

33. UV-Vis Spectra of Conjugated Aldehydes

Build and perform Geometry Optimization calculations for the following molecules. Using the resulting geometry, perform UV-Vis Spectra calculations for each molecule.



The first excited state (A") corresponds to a forbidden $n \rightarrow \pi^*$ transition and is therefore extremely weak. The second excited state (A') corresponds to an allowed $\pi \rightarrow \pi^*$ transition and is strongly absorbing. Compare the computed absorption maximum to the experimentally observed maximum in a table with columns for molecule, computed maximum, experimental maximum, and difference. Comment on any trends that are observed.

34. Excited State Optimization and Vibrational Frequencies of Formaldehyde

Build ground state (S_0) formaldehyde, H₂CO, and perform a Hartree-Fock 6-31G(d) Geometry Optimization calculation. Using the resulting geometry, perform a Vibrational Frequencies calculation at the same level of theory.

The first excited singlet state (S_1) of formaldehyde is pyramidal. Build S_1 formaldehyde, and move the O atom out of the molecular plane by adjusting the O-H-H-C dihedral angle to 20 degrees. Perform a Hartree-Fock 6-31G(d) Geometry Optimization calculation, but use the Advanced Options dialog box and check the Excited State option. Using the resulting geometry,

perform a Vibrational Frequencies calculation at the same level of theory and with Excited State option checked.

Mode	Description	S_0 Scaled Frequency (cm ⁻¹)	S_1 Scaled Frequency (cm ⁻¹)	S_1 Literature Frequency (cm ⁻¹)
ν_1	sym CH stretch			2846
v ₂	CO stretch			1183
v ₃	CH ₂ bend			1293
ν_4	out-of-plane bend			
v ₅	antisym CH stretch			2968
ν_6	CH ₂ rock			904

Complete the following table, using the scaling factor of 0.8929 for Hartree-Fock 6-31G(d) frequency calculations.

Which vibrational modes undergo the largest change upon electronic excitation? Offer an explanation for your result, noting that S_1 is pyramidal and that the $S_0 \rightarrow S_1$ electronic transition is an $n \rightarrow \pi^*$ transition.

N. Solutions

35. Solvation Energies of Cations

Build the ammonium cation, NH_4^+ , and perform a Geometry Optimization calculation. Be sure to set the charge appropriately for a cation. Using the resulting geometry, perform another Geometry Optimization calculation, but use the Advanced Options to select water as the solvent.

Repeat the gas phase and aqueous calculations for tetramethyl ammonium cation, N(CH₃)₄⁺.

If using WebMO Pro, select the four jobs in Job Manager and click the **Spreadsheet** button to obtain an immediate comparison among the four calculations. Otherwise, view the results of each job.

Solvation energy is the energy change upon solvation, i.e., $E_{solvation} = E_{solution} - E_{gas}$. The experimental solvation energies for NH_4^+ and $N(CH_3)_4^+$ are -88 kcal/mol and -60 kcal/mol, respectively. Make a table with columns for molecule, gas phase energy, solution energy, calculated solvation energy, and experimental solvation energy. Comment on the accuracy of the solvation model being used.

36. Solvation Energy of Glycine and its Zwitter Ion

The amino acid glycine has a zwitter ion isomer, in which the carboxylic acid proton is transferred to the amino group.



Build glycine and perform a Geometry Optimization calculation. Using the resulting geometry, perform a Molecular Energy calculation at the same level of theory but using the Advanced Options to select water as the solvent.

Repeat the gas phase Geometry Optimization and aqueous Molecular Energy calculations for the zwitter ion.

If using WebMO Pro, select the four jobs in Job Manager and click the **Spreadsheet** button to obtain an immediate comparison among the four calculations. Otherwise, view the results of each job.

Solvation energy is the energy change upon solvation, i.e., $E_{solvation} = E_{solution} - E_{gas}$. Make a table with columns for molecule, gas phase energy, solution energy, and solvation energy.

Which isomer is more stable in the gas phase? Which isomer is more stable in water? Comment on the reason for the difference in solvation energies between the two isomers.

O. Electrostatic Potential

37. Electrostatic Potential Surface of Imidazole (Pro)

Imidazole has two basic sites on the nitrogen atoms. The more basic site can be determined by locating the region of negative charge density around the molecule.



Build imidazole, $C_3H_4N_2$, and optimize the geometry with a PM3 calculation. View the result, click New Job Using This Geometry, and perform a Molecular Orbitals calculation at the same level of theory. On the job results page, view the Electrostatic Potential, which opens the

MOViewer application. The electrostatic potential is painted onto an electron density isosurface, with red being negative and blue being positive. In Edit: Preferences..., adjust the Opacity of the surface to about 70%.

Use the electrostatic potential image to determine which nitrogen is more basic, i.e., would more likely attract a proton.

Confirm your prediction by computing Geometry Optimization calculations of the NH protonated cation and for the N protonated cation and comparing their energies.

P. Frontier Density

38. Nucleophilic (LUMO) Frontier Density (Pro)

Carbonyl groups undergo nucleophilic attack, which could in principle occur at either the carbon or at the oxygen atom. The nucleophilic attack site is a region where the nucleophile can donate its electron density to the carbonyl group. The site and orientation of nucleophilic attack can be inferred by viewing the carbonyl group LUMO, or directly viewed by visualizaing the LUMO density.

Build acetone, C_3H_6O , and optimize the geometry with a Hartree-Fock STO-3G calculation. View the result, choose New Job Using This Geometry, and perform a Molecular Orbitals calculation at the same level of theory.

On the job results page, view the LUMO (Lowest Unoccupied Molecular Orbital), which opens the MOViewer application. Infer whether the largest contribution comes from the carbonyl carbon or carbonyl oxygen.

View the Nucleophilic (LUMO) Frontier Density. The Frontier Density is painted onto an electron density isosurface, with red being smallest and blue being the largest. In Edit: Preferences..., adjust the Opacity of the surface to about 70%. Which atom is most likely to be attacked by a nucleophile? Is the attack likely to come from in the plane of the carbonyl group, or from out of the plane?

39. Electrophilic (HOMO) Frontier Density (Pro)

Enolate anions undergo electrophilic attack, which can occur at either the oxygen atom or at the beta-carbon atom.



Build ethyl enolate, by first building the corresponding alcohol and then deleting the alcohol H atom. Optimize the geometry with a Hartree-Fock STO-3G calculation. View the result, choose New Job Using This Geometry, and perform a Molecular Orbitals calculation at the same level of theory.

On the job results page, view the HOMO (Highest Occupied Molecular Orbital), which opens the MOViewer application. Note that the electron density is delocalized across oxygen-carbon π system.

View the Electrophilic (HOMO) Frontier Density. The Frontier Density is painted onto an electron density isosurface, with red being smallest and blue being the largest. In Edit: Preferences..., adjust the Opacity of the surface to about 70%. Which atom is most likely to be attacked by an electrophile?

Q. Independent Project

40. Independent Computational Chemistry Project

Propose and carry out an independent computational chemistry project. The topic may be an extension of one of the above assignments, related to an ongoing research project, or based on a journal article or a textbook example.

A. Proposal. Identify the chemical system(s) to be studied, any systematic variables to be investigated, a list of the specific calculations that will be performed, the type of results expected from the calculations (energies, structures, orbitals, thermodynamic values, kinetics values, etc.), and any experimental data to which the computed results can be compared. Limit the proposal to 1 page or less. The proposal will be evaluated for choice of topic and thoroughly anticipating the calculations used in the project. Feedback concerning the proposed calculations will be offered.

B. Oral presentation. Make a 10 minute oral presentation and answer questions about your talk. Use Powerpoint or equivalent presentation program for the talk. A possible outline might be: Title, Statement of Problem, Numerical Results (in Tables and/or Plots), Visual Results, Interpretation, Comparison to Experiment, Conclusion. Use molecular pictures to explain your points, and keep tables simple enough to easily understand. The oral presentation will be evaluated for content, clarity and organization, enthusiasm, and observing the time limit.

C. Written report. Prepare a written report describing your project. The report should typically be 3-5 pages of written text, plus tables and figures. The report will consist of a title, introduction, outline of calculations, results, discussion, conclusion and references. The calculations will be evaluated for appropriateness and correctness. The report will be evaluated for spelling and grammar, overall clarity, use of tables and/or figures to present results, and effectiveness of discussion.

8. Appendices

A. Installing WebMO

1. Obtain a WebMO license from http://www.webmo.net. A license number and download password will be emailed to you.

2. Download WebMO to your PC.

3. Upload the WebMO archive from your PC to your unix (Linux, IRIX, AIX, Solaris, etc.) web server. Do **not** uncompress the archive on your PC before uploading!

- 4. Login to your web server account, uncompress, and untar the WebMO archive.
 - \$ gunzip WebMO.3.3.00x.tar.gz
 - \$ tar xvf WebMO.3.3.00x.tar
- 5. Run the setup script.
 - \$ cd WebMO.install
 - \$ perl setup.pl

6. Follow the directions that are given in the setup script:

- Enter WebMO license number when prompted
- Select the appropriate Perl binary
- Select CGI directory and URL
- Select HTML directory and URL
- Select directory for user files

After the distribution files are copied, the command line portion of WebMO setup is complete.

7. Follow the URL given at the end of setup process and continue with the on-line WebMO configuration:

- Login as user 'admin' with an empty password.
- Reset the admin password when prompted.
- Register your copy of WebMO when prompted.
- If the registration process fails (e.g., due to no internet connectivity), login again from the URL at the end of the setup process as user 'admin' with the new password.
- Click 'System Manager' and confirm that locations of various system utilities have been correctly set (this should have already been completed automatically).
- Click 'Return to Admin' to return to the WebMO administration page.
- Click 'Interface Manager' and enable the interfaces to any computational chemistry packages that you have installed on your system. Click the 'Enable' button to enable an interface that is currently disabled.

- Click 'Return to Admin' to return to the WebMO administration page.
- Click '*interface_name* Manager' to configure any interfaces that were enabled in the Interface Manager. Make any necessary changes in the interface configuration and then click submit to commit the changes.
- Click 'Return to Admin' to return to the WebMO administration page.
- Click on the 'User Manager' and then the 'New User' button to create WebMO users. Create at least one user.
- Click 'Return to User Manager' to return to the user manager.
- Click 'Return to Admin' to return to the WebMO administration page.
- Setup is complete. Click the 'Logout' button to logout of the WebMO administration page.

8. Login as the WebMO user that you created. In the job manager, click 'Create New' to run a test job.

9. If you have not yet installed any computational chemistry programs on your unix computer, see the separate support pages at http://www.webmo.net/support for installing binary or source versions of Gaussian, MOPAC, and GAMESS. Then enable, configure, and test them.

B. Upgrading WebMO

1. Log into WebMO as admin and click the Version Manager. Note:

- your WebMO license number
- the location of the WebMO globals.int file

These are needed to download the WebMO update and to install the update, respectively.

2. Download the most recent version of WebMO from http://www.webmo.net to your PC. If you have misplaced your WebMO password, enter the license number from the previous step with a password of '?' on the download page, and your password will be automatically emailed to you.

3. Upload the WebMO archive from your PC to your web server.

4. Backup your current WebMO installation. For example,

\$ tar cvf webmo_backup.tar {cgiBase} {htmlBase} {userBase}
where {cgiBase}, {htmlBase}, and {userBase} are specified in the WebMO globals.int
configuration.

5. Login to your web server account, uncompress, and untar the WebMO archive.

- \$ gunzip WebMO.3.3.xxx.tar.gz
- \$ tar xvf WebMO.3.3.xxx.tar
- 6. Run the upgrade script.

8. Appendices

```
$ cd WebMO.install
$ perl upgrade.pl
```

7. Follow the directions that are given in the setup script and specify the absolute location of your globals.int file. After the distribution files are copied, the command line portion of WebMO upgrade is complete.

8. If you are upgrading WebMO Pro and have configured any remote servers, login in as 'admin', click the Remote Server Manager, select the remote server and click Change, and click the Upgrade button to copy the new scripts to the remote server.

C. Installing MOViewer (Pro)

- 1. Perform a Molecular Orbital calculation for any molecule, e.g., H₂O.
- 2. View the job results and scroll down to the bottom of the Molecular Orbitals results.
- 3. Click the 'Help Viewing MOs' link.

4. Download MOViewer Setup program (InstallMOViewer.exe) and save the file to the client computer when prompted.

5. Run the InstallMOViewer.exe program on the client computer.

6. Click 'Next', read and agree to the terms of the license agreement, select an installation location, select a 'Typical' installation type, and wait for the installation to complete.

7. If necessary, restart your computer when prompted.

Notes

Notes

"WebMO is a simple, Web browser-based interface for using popular chemistry software packages, such as Mopac and Gaussian. You draw the molecule's structure, and the output – including the molecule's transition states and infrared and nuclear magnetic resonance spectra – appears in an easy-to-understand format."

Science, August 10, 2001

"WebMO is a Web-based interface to computational programs such as Gaussian, Gamess, and Mopac. The user draws a molecule using a 3-D editor, sets up the calculation, submits the job, and views the results graphically, all within a standard Web browser. WebMO is simple enough for an undergraduate computational chemistry curriculum and flexible enough for computational chemistry research."

C&E News, April 8, 2002



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www.webmo.net