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.
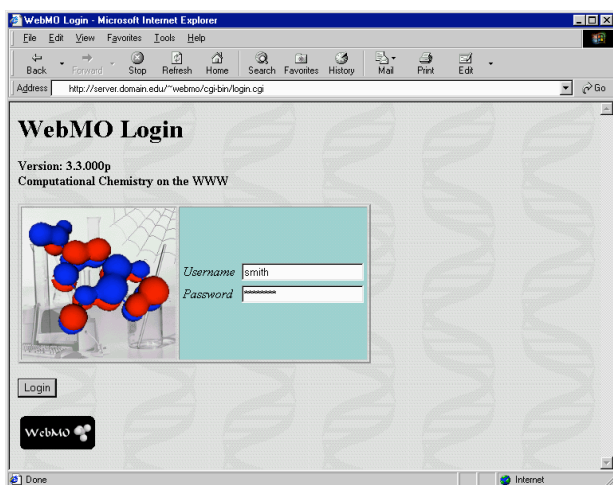
WebMO Login Page

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.

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
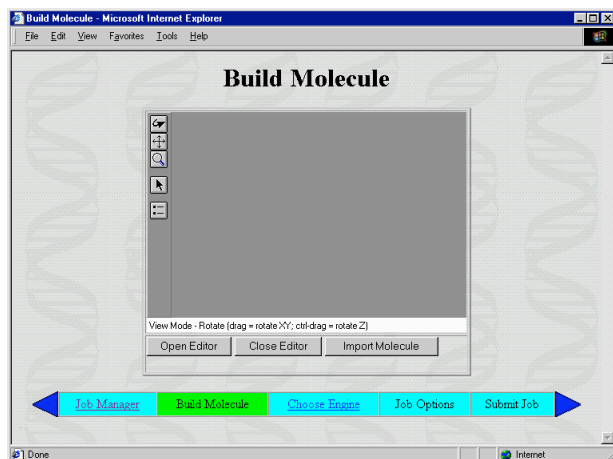
WebMO Build Molecule Page

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 ⬚ 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... (⬚). 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 (⬚).

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To further adjust the geometry (bond length, bond angle, or dihedral angle) of the molecule, choose Tools: Adjust ([icon]) 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 ([icon]), Adjust: Bond Angle ([icon]), or Adjust: Dihedral Angle ([icon]), 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.)
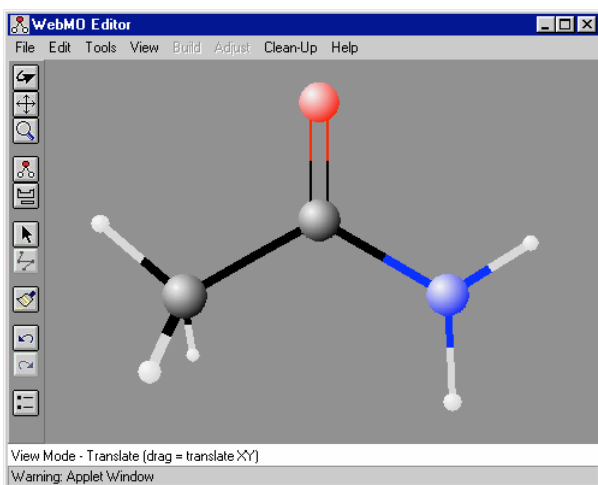
WebMO 3-D Molecular Editor

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).

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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.
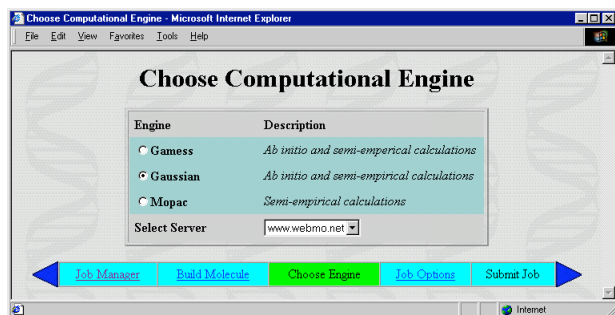
WebMO Choose Computational Engine Page

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.)
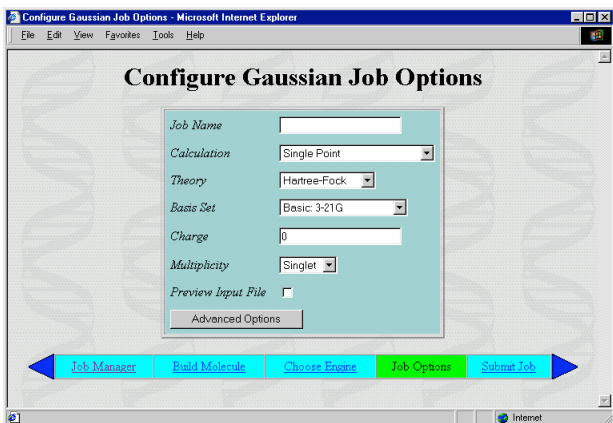
WebMO Configure Job Options Page
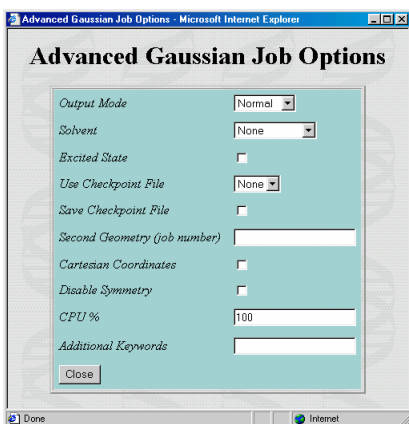
WebMO Advanced Options Page

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.

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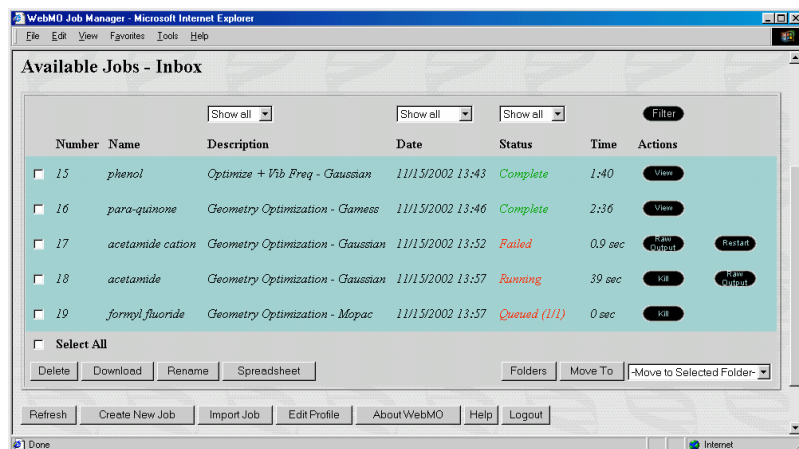
WebMO Job Manager with Completed, Failed, Running, and Queued Jobs

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

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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.

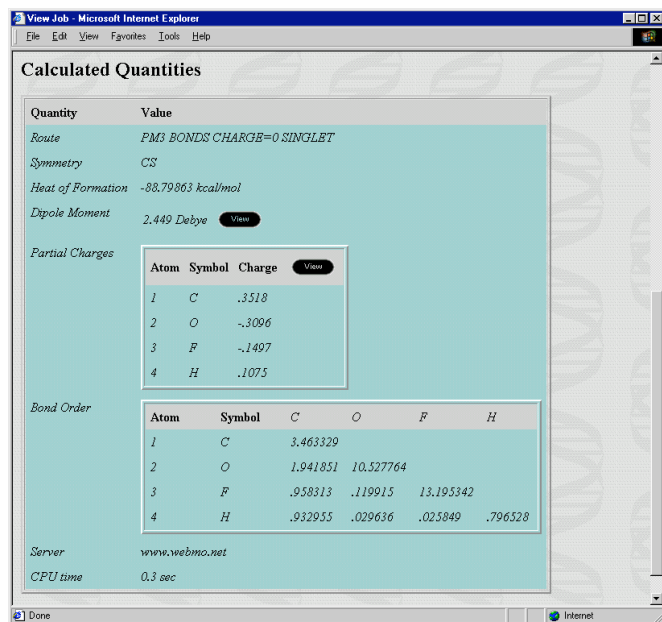The final geometry may be exported into a variety of formats using the Export Molecule button.

The complete output file of the computational chemistry program may be viewed by clicking the Raw Output button.
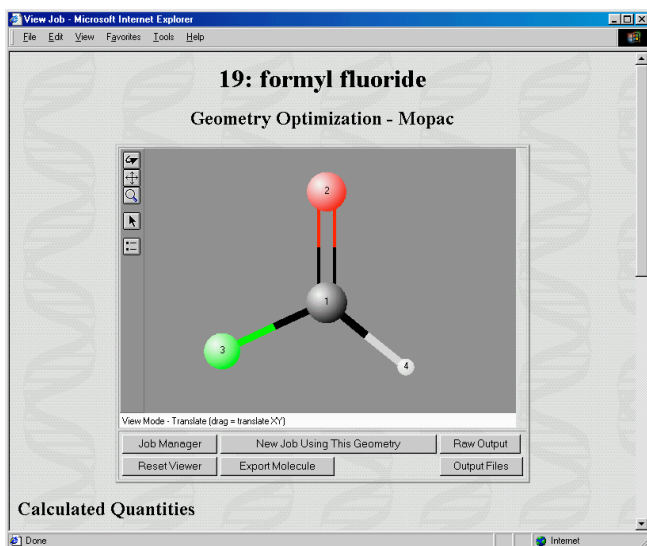
WebMO View Job Page (part 1/2)

1. WebMO Introduction

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.