WebMO: Web-based, state-of-the-art, and cost effective computational chemistry

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Abstract

WebMO (www.webmo.net) is a free web-based interface to popular computational chemistry programs. WebMO permits users to build 3-D molecular structures, submit multiple jobs, monitor job progress, and view text and graphical results, all from within a standard web-browser. WebMO overcomes the resource and accessibility challenges associated with traditional GUI interfaces since it is installed on a single server, requires no installation on student computers, and is available anywhere on the internet. WebMO is simple enough for undergraduate computational chemistry courses and flexible enough for computational chemistry research.

Computational Chemistry in Education

Computer modeling has become widely recognized as the third pillar of science, together with experiment and theory.[1] Computation allows scientists to model realistic problems which do not have analytical or simple solutions, and allows scientists to answer questions that are difficult (either for technical or financial reasons) to address by conventional experimental means. In chemistry, computational modeling is used extensively in academic research and by the pharmaceutical industry. Computational chemistry provides insight into chemical structure, interactions, and reactivity, which in turn permits the prediction of chemical behavior. A high fraction of chemistry research articles include some modeling to analyze and interpret results, and modeling can be used to predict promising leads for subsequent experimental investigation.

Some progress has been made to introduce computation into the undergraduate chemistry curriculum, often as an isolated laboratory experience or a specialized upper-level course. But computational chemistry has not yet become infused throughout undergraduate chemistry education, like chemical synthesis or spectroscopic characterization. Many of the technical issues associated with scientific computing have been recently overcome. For example, typical student laptop computers have more computing power than supercomputers of 15 year ago[2] and high-end research computers of a few years ago. Graphical user interfaces and menu systems make computers much more usable than before. Current computer codes[3] can accurately compute chemical energies to within a few kcal/mole and vibrational frequencies to within 20 cm^{-1}. A wide variety of exercises have been developed for use in undergraduate chemistry courses.[4]

Yet despite the value of chemical computation and the technical solutions to its application, three significant barriers exist to the widespread use of computational chemistry in education:

- **Ease-of-use:** State-of-the-art computer codes are difficult for chemistry students and faculty to use. This issue has typically been resolved by installing both a program and a graphical interface on the user's computer, e.g., Gaussian/Gaussview,[5] Spartan,[6] CAChe,[7] PCModel,[8] NWChem/ECCE.[9] Yet significant issues remain with regard to support of multiple computing platforms (e.g., Windows, Macintosh, and Unix) and support of students wishing to run software on their own computers.
- **Resources (time and money):** If a school sets up a computational chemistry laboratory, significant costs are associated with the purchase of computer hardware and the associated software licenses for each individual workstation. In addition, it takes significant time to install and maintain each installation.
- **Accessibility:** Users must gain physical access to the computers inside a computational chemistry laboratory and cannot use the programs from another location or their own laptop.

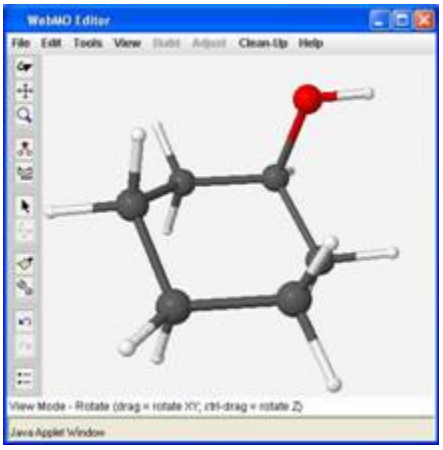
WebMO fully solves these ease-of-use, resource, and accessibility challenges. Molecules are drawn with a 3-D editor, selections are made from menu systems, calculations are run using popular state-of-the-art computer codes, and results are viewed graphically or in formatted tables. WebMO provides an easy-to-use, uniform interface to nearly all popular computational chemistry packages. Only one server computer and one license for commercial software is needed, dramatically reducing the hardware and software costs. Since no software is installed on client computers, time-consuming maintenance issues are also minimized. WebMO requires only a web browser on any computer (Windows, Macintosh, Unix) connected to the internet, making computational chemistry universally accessible to anyone from any location. For example, students can do computational chemistry exercises from their dorm rooms using their laptop computers.

WebMO Interface to Computational Chemistry

WebMO is a web-based interface for computational chemistry programs.[10] 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 installs on a single unix computer (Linux, Macintosh OS X, Solaris, Irix, etc.), after which it is accessed and administered from a standard web browser from any computer (Windows, Macintosh, Unix). And most importantly, **WebMO is free**. A commercial add-on to the free package called WebMO Pro is also available for advanced users.

After logging into WebMO, the user can draw a molecule using a **3-D editor** or import a structure from a variety of formats. The molecular editor provides for adding missing hydrogen atoms using organic chemistry rules, idealizing the geometry using VSEPR rules, inserting molecular fragments, manually adjusting the molecular geometry, and minimizing the molecular energy using molecular mechanics. Creating a molecule by clicking to insert atoms and dragging to insert bonds is extremely intuitive and requires very little student training. Advanced users can specify the Z-matrix used to represent the molecular geometry, as well as the internal coordinates to be fixed, optimized, and/or scanned.

After choosing one of the installed computational engines, the **calculation type** (Geometry Optimization, Vibrational Frequencies, Molecular Orbitals, etc.) is selected from a dropdown menu. Common job options (Theory, Basis Set, Charge, Multiplicity) may be specified, although reasonable defaults are provided. Additional options (Symmetry, Solvent, Coordinate System, Electronic State, etc) may also be specified. Prior to submitting the job, the user can examine and directly edit the job input file if desired, which gives complete control over the job details and provides an opportunity to learn how to construct input files for different programs.

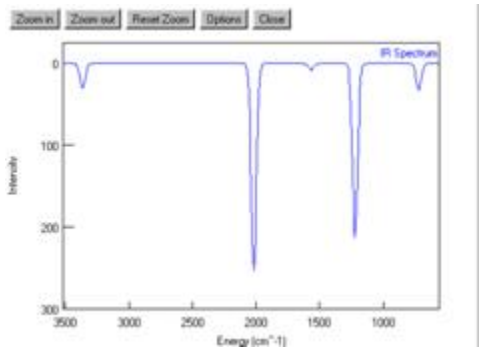


WebMO 3-D editor

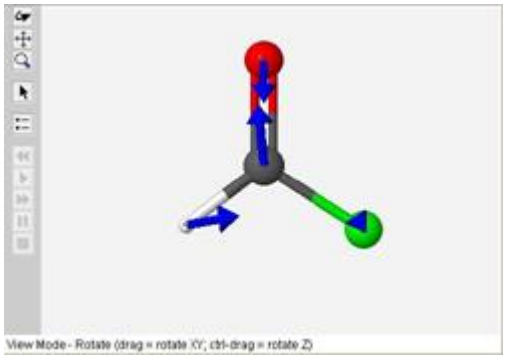
Job options page

When a job is submitted, it is sent to the WebMO **job queue** where it is run in turn at the first available opportunity. WebMO Pro also allows jobs to be run on a remote computer or using the system's batch system (PBS, NQS, Sun Grid Engine). While running, the job is continuously monitored and the partially complete raw output can be examined.

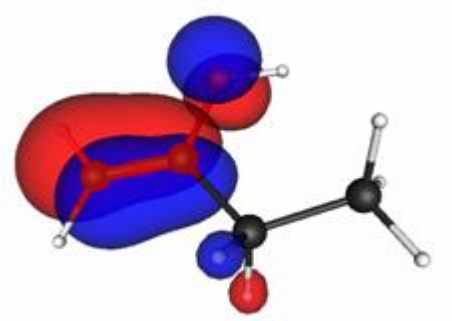
When completed, the results can be **visualized in 3-D**, and bond lengths, bond angles, and dihedral angles can be measured. Partial charges and the dipole moment are both tabulated and displayed visually. Vibrational frequency calculations animate the normal modes and display an infrared spectrum. UV-VIS and NMR spectra can also be displayed. WebMO Pro also displays coordinate scans, molecular orbitals and their dependent functions, and spreadsheet summaries that can compare different calculations. Molecular geometries can also be exported into mol, pdb, or xyz files for use by other applications.



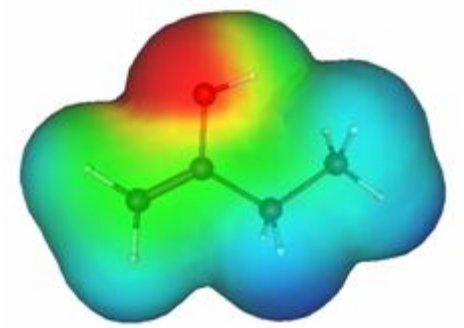
Infrared spectrum



Normal mode



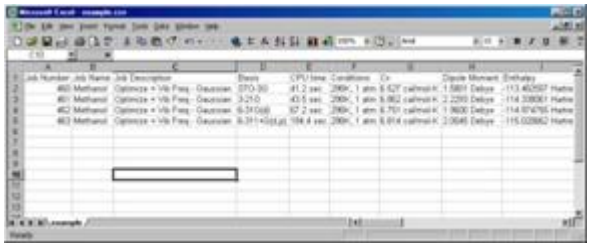
Molecular orbital



Electrostatic potential

Queued, running, and completed jobs are **managed** using the Job Manager, which includes a variety of features including uploading and downloading jobs, setting user preferences, and user-defined folders for organizing jobs in WebMO Pro.

A variety of **administrative tools** are provided, such as setting of job time limits, creation of student accounts from Excel lists, designation of groups of students that correspond to different classes and/or different privilege levels, filtering jobs by user or group, viewing jobs, and management of jobs. These features are designed to permit a single instance of WebMO Pro to be used by multiple faculty members who oversee different classes of students. The WebMO administrator can also configure WebMO settings, check for updates, and configure settings for individual computational programs using the web interface.



Job manager Spreadsheet summaries

Since WebMO is web-based, no software is installed on a user's computer. Only the web browser that comes with every Windows, Macintosh, or Linux computer is needed to use WebMO. Thus, prospective users can visit the WebMO Working Demo at

http://www.webmo.net/demo/

and try WebMO just as easily as visiting any other website.

Capabilities of WebMO

WebMO supports a variety of popular, state-of-the-art computer programs:

- Gamess 1998+
- Gaussian 94/98/03
- Molpro 2002+
- Mopac 7/93/200x
- Nwchem 4.6+
- Qchem 2.1+
- Tinker 4.2+

and works fully with a variety of web browsers, including:

- Internet Explorer 4.0+ (Windows)
- Safari 1.2+ (Macintosh)
- Mozilla Firefox (Windows, Macintosh, Unix)

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
- Bond orders and partial charges
- Geometry optimization
- Transition state optimization
- Saddle calculation
- Vibrational frequencies, spectra, and motions
- UV-VIS frequencies and spectra
- NMR frequencies and spectra
- Thermochemistry
- IRC calculation
- Molecular orbitals*
- Natural bond orbitals*
- Electron density isosurfaces*
- Electrostatic potentials*
- Nucleophilic and electrophilic frontier orbital densities*
- Coordinate scan*

(* indicates WebMO Pro feature)

Cost of WebMO

Since WebMO, the linux operating system, and some of the underlying computational engines are free, a very capable computational chemistry system can be assembled at

little to no cost. Should one wish to license commercial software, purchase a WebMO Pro license, or purchase state-of-the-art hardware, the cost will increase. Regardless, the total cost of a WebMO system will typically be many times less than a computer lab outfitted with computational chemistry software, and it will typically serve many more students. The range of typical costs associated with WebMO is shown below.

Item	Cost
PC (1GHz, 256MB, 40GB minimum)	$ 0 - 1000
Linux OS	$ 0 - 100
Computational engines (Gamess, Gaussian, Molpro, Nwchem, Mopac, Qchem, Tinker)	$ 0 - 2500
WebMO or WebMO Pro	$ 0 - 995
TOTAL	**$ 0 - 4600**

Conclusions

Computational chemistry is becoming an increasingly important part of every chemist's training. Although today's computer hardware and software are capable of high accuracy chemical calculations, concerns about ease-of-use, time, money, and accessibility are still preventing the widespread use of computational chemistry in the undergraduate curriculum. WebMO is a web-based interface to computational chemistry that solves these problems. Students are able to use a web browser on their personal computers to easily setup and run state-of-the art calculations using a graphical interface. WebMO installs on a single server computer, greatly reducing hardware, software, and maintenance costs. WebMO can be accessed from any computer on the internet, resulting in universal accessibility. Thus, undergraduate students in any chemistry course, from general chemistry through undergraduate research, can readily use WebMO to perform computational chemistry calculations as part of their chemistry education.

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