



WebMO

Jack Smith

Center for Environmental, Geotechnical and Applied Science
Marshall University

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Division of Science and Research
WV Higher Education Policy Commission

WVU HPC Summer Institute
June 20, 2014



Outline

- Accessing WebMO on Marshall's HPC cluster
- Overview of WebMO capabilities
- Building molecules
- Submitting jobs
- Optimizing a geometry
- Electronic properties
- Visualizing orbitals, densities, and electrostatic potential
- IR spectrum and animating the vibrational modes
- UV-Vis spectrum
- Geometry scan, transition state, and reaction pathway
- Future topics
- Exercises



Accessing WebMO

- Non-Marshall people will first need to apply for MU ID
 - Contact Ed Aractingi at aractingi1@marshall.edu for form
- Apply for account on HPC cluster
 - Use form at: <http://bit.ly/eDHJEU>
 - Select 'Jack Smith' as sponsor
 - Check 'yes' for access to WebMO on form
- Already have an HPC cluster account, but no WebMO access?
 - Contact Jack Smith at smith1106@marshall.edu for WebMO access
- Log in to WebMO with web browser
 - <http://biggreen.marshall.edu/~webmo/cgi-bin/webmo/login.cgi>
 - Use your regular MU login credentials
 - Browser needs recent Java plug-in for 3D editor
- WebMO now available as an app for iPad (\$4.99)
 - Still needs access to WebMO account on cluster



Accessing WebMO

*** *as workshop student only* ***

- Log in to WebMO with web browser
 - <http://biggreen.marshall.edu/~webmo/cgi-bin/webmo/login.cgi>
 - Use username provided by instructor (e.g., *student01*)
 - Password will also be provided by instructor
 - Accounts will expire at the end of the HPC Summer Institute
 - Browser needs recent Java plug-in for 3D editor



Accessing WebMO

Login

The screenshot shows a web browser window with the title 'WebMO Login'. The address bar displays the URL 'muci-train01.marshall.edu/~webmo/cgi-bin/webmo/login.cgi'. The browser's bookmark bar is visible with various links like Google, Toodledo, Social Media, Mail, Bills Online, WesBancoNet, MATRIC, Marshall, TeraGrid, UICDS, TV & Movies, MobileMe, and Other bookmarks. The main content area has a blue background. At the top left, it says 'WebMO Login' in white, followed by 'Version: 10.1.002e' and 'Jack Smith'. Below this is a login form with a molecular model image on the left. The form contains two input fields: 'Username' with the text 'smith1106' and 'Password' with masked characters '*****'. Below the form is a 'Login' button. At the bottom left of the page is a 'WebMO' logo.

WebMO Login

Version: 10.1.002e
Jack Smith

Username

Password

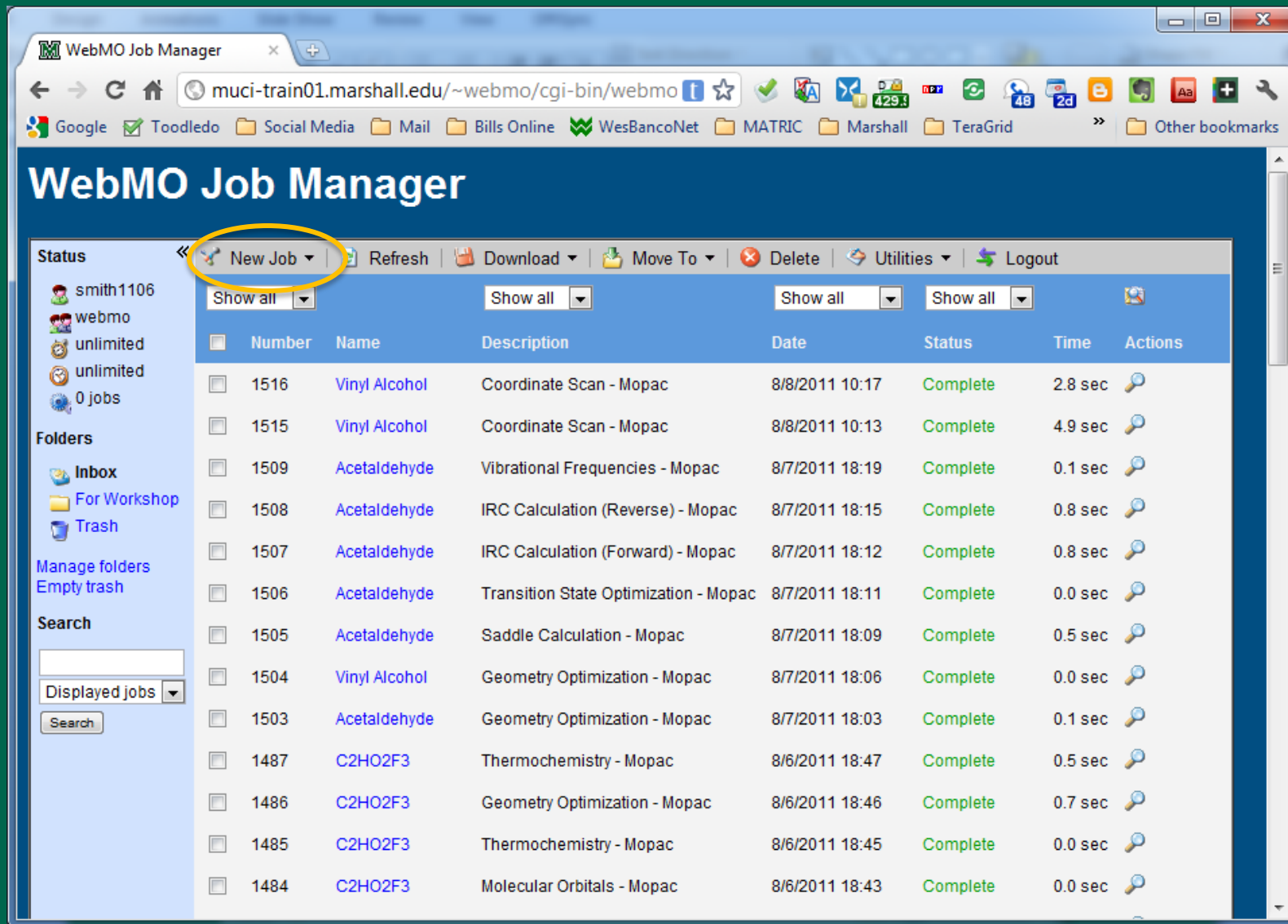
Login

WebMO

<http://biggreen.marshall.edu/~webmo/cgi-bin/webmo/login.cgi>

Accessing WebMO

Job Manager



WebMO Job Manager

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

Filters: Show all, Show all, Show all, Show all

Number	Name	Description	Date	Status	Time	Actions
1516	Vinyl Alcohol	Coordinate Scan - Mopac	8/8/2011 10:17	Complete	2.8 sec	
1515	Vinyl Alcohol	Coordinate Scan - Mopac	8/8/2011 10:13	Complete	4.9 sec	
1509	Acetaldehyde	Vibrational Frequencies - Mopac	8/7/2011 18:19	Complete	0.1 sec	
1508	Acetaldehyde	IRC Calculation (Reverse) - Mopac	8/7/2011 18:15	Complete	0.8 sec	
1507	Acetaldehyde	IRC Calculation (Forward) - Mopac	8/7/2011 18:12	Complete	0.8 sec	
1506	Acetaldehyde	Transition State Optimization - Mopac	8/7/2011 18:11	Complete	0.0 sec	
1505	Acetaldehyde	Saddle Calculation - Mopac	8/7/2011 18:09	Complete	0.5 sec	
1504	Vinyl Alcohol	Geometry Optimization - Mopac	8/7/2011 18:06	Complete	0.0 sec	
1503	Acetaldehyde	Geometry Optimization - Mopac	8/7/2011 18:03	Complete	0.1 sec	
1487	C2HO2F3	Thermochemistry - Mopac	8/6/2011 18:47	Complete	0.5 sec	
1486	C2HO2F3	Geometry Optimization - Mopac	8/6/2011 18:46	Complete	0.7 sec	
1485	C2HO2F3	Thermochemistry - Mopac	8/6/2011 18:45	Complete	0.0 sec	
1484	C2HO2F3	Molecular Orbitals - Mopac	8/6/2011 18:43	Complete	0.0 sec	



WebMO Capabilities

- Supports many computational engines
 - **GAUSSIAN, GAMESS, MOPAC, Tinker, NWChem,**
Quantum Espresso, VASP, MolPro, PQS, PSI, QChem
- GUI is completely browser-based (+Java 3D)
- Built-in 3D molecular editor
- Batch (PBS, SGE, built-in) job submission and management
- Visualization of results
- Tabulation of results
- Upload/download files from/to desktop
- See WebMO website for more info:
<http://www.webmo.net>



WebMO Capabilities

Calculation Types

- Single-point energy calculation
- Geometry optimization
- Electronic properties
 - Molecular orbitals, partial charges, dipole moment
- Geometry scan
 - Conformational analysis, reaction coordinates
- IR spectrum (vibrational analysis)
- UV-Vis spectrum (excitations)
- NMR spectrum (chemical shifts, shielding)
- Thermochemistry and “model chemistries”



WebMO Capabilities

Levels of Theory

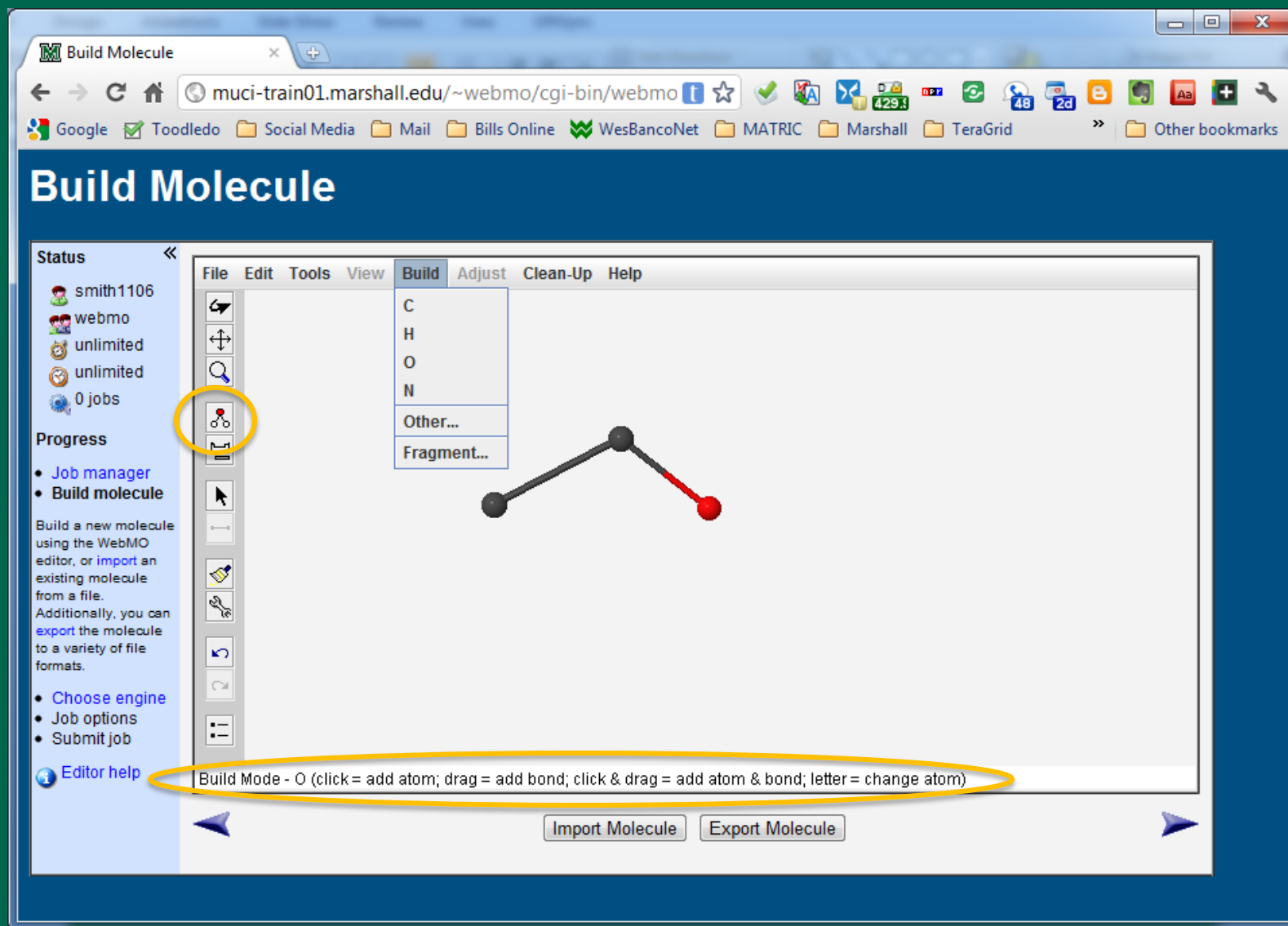
- | | |
|---|-----------------|
| • Molecular Mechanics | Tinker |
| • No electrons! No breaking or forming bonds! | |
| • Forcefields: MM3,... | |
| • Semi-empirical (Quantum Mechanical) | MOPAC |
| • HF with parameterized integrals | |
| • Fit to Heats of Formation | |
| • Density Functional Theory | GAMESS |
| • No wavefunction! | NWChem |
| • Approximate exchange-correlation: B3LYP,... | <i>GAUSSIAN</i> |
| • <i>Ab initio</i> (Wave Function) | : |
| • HF – no electron correlation! | |
| • Correlation: CI, MP, MBPT, CC,... | |



Building Molecules

- Use **build tool** to click and drag atoms and bonds
- Use **build menu** (or periodic table) to change element or add a pre-defined fragment
- Use right-click **context menu** to change element hybridization/charge or bond order
- Use **cleanup** tool/menu to add Hydrogens, assign hybridizations, and clean up geometry
- Use **rotate**, **translation** and **zoom** tools to manipulate view
- Use **adjust tool** and shift-click to select atoms, bonds, angles or dihedrals and modify their values
- Check **status line** for current tool/view mode and available mouse/keyboard options

Building Molecules



The screenshot shows a web browser window with the URL `muci-train01.marshall.edu/~webmo/cgi-bin/webmo`. The page title is "Build Molecule". The interface includes a status bar on the left, a main workspace with a menu and toolbar, and a bottom status bar.

Status Bar (Left):

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs
- Progress**
 - Job manager
 - Build molecule
- Build a new molecule using the WebMO editor, or **import** an existing molecule from a file. Additionally, you can **export** the molecule to a variety of file formats.
- Choose engine
- Job options
- Submit job
- Editor help

Main Workspace:

- Menu:** File, Edit, Tools, View, **Build**, Adjust, Clean-Up, Help. The "Build" menu is open, showing options: C, H, O, N, Other..., and Fragment....
- Toolbar:** Contains icons for undo, redo, pan, zoom, and atom/bond addition. The atom addition icon (a red circle with a plus sign) is circled in yellow.
- Canvas:** Displays a molecular structure consisting of two black spheres (Carbon) connected by a single bond, with a red sphere (Oxygen) attached to one of the black spheres.

Bottom Status Bar:

Build Mode - O (click = add atom; drag = add bond; click & drag = add atom & bond; letter = change atom)

Buttons: Import Molecule, Export Molecule

Building Molecules

Build Molecule

← → ↺ ↻ ↵ ↶ ↷ ↸ ↹ ↺ ↻ ↵ ↶ ↷ ↸ ↹

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

Build Molecule

Status

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs

Progress

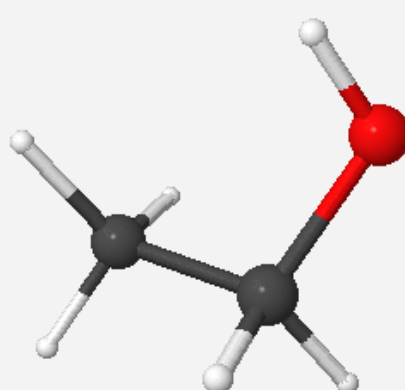
- Job manager
- Build molecule

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

- Choose engine
- Job options
- Submit job

[Editor help](#)

File Edit Tools View Build Adjust Clean-Up Help



View Mode - Translate (drag = translate XY)

Import Molecule Export Molecule

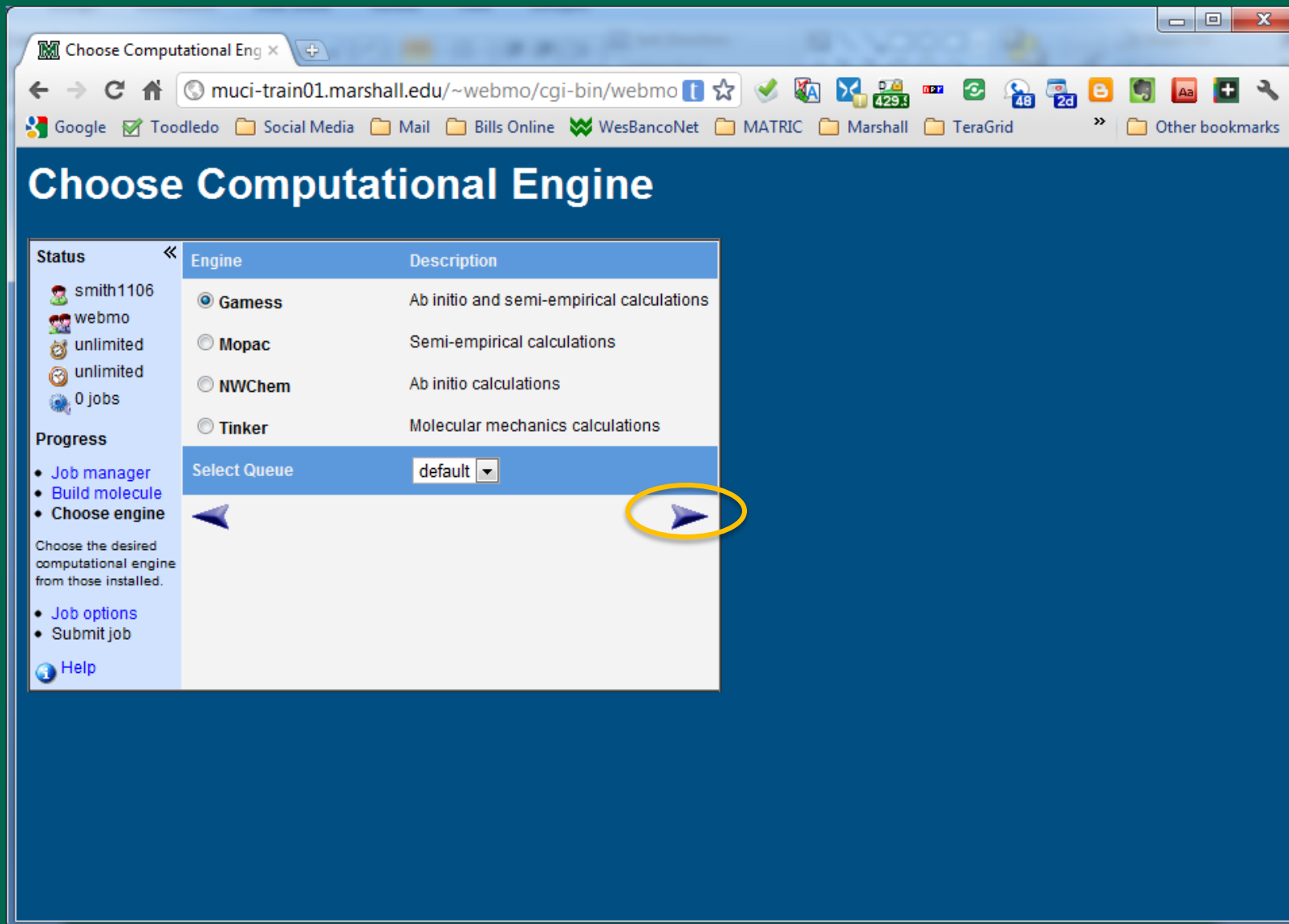


Submitting Jobs

- Choose Computational Engine
 - GAMESS, Gaussian, NWChem, MOPAC, Tinker
- Configure Job Options
 - Name
 - **Calculation Type**
 - Level of Theory
 - DFT Functional (for DFT)
 - Basis Set
 - Charge
 - Spin Multiplicity
- Submit to queue
- Monitor in Job Manager

Submitting Jobs

Choose Computational Engine



Choose Computational Eng x

muci-train01.marshall.edu/~webmo/cgi-bin/webmo

Choose Computational Engine

Status <<

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs

Progress

- Job manager
- Build molecule
- Choose engine
- Job options
- Submit job
- Help

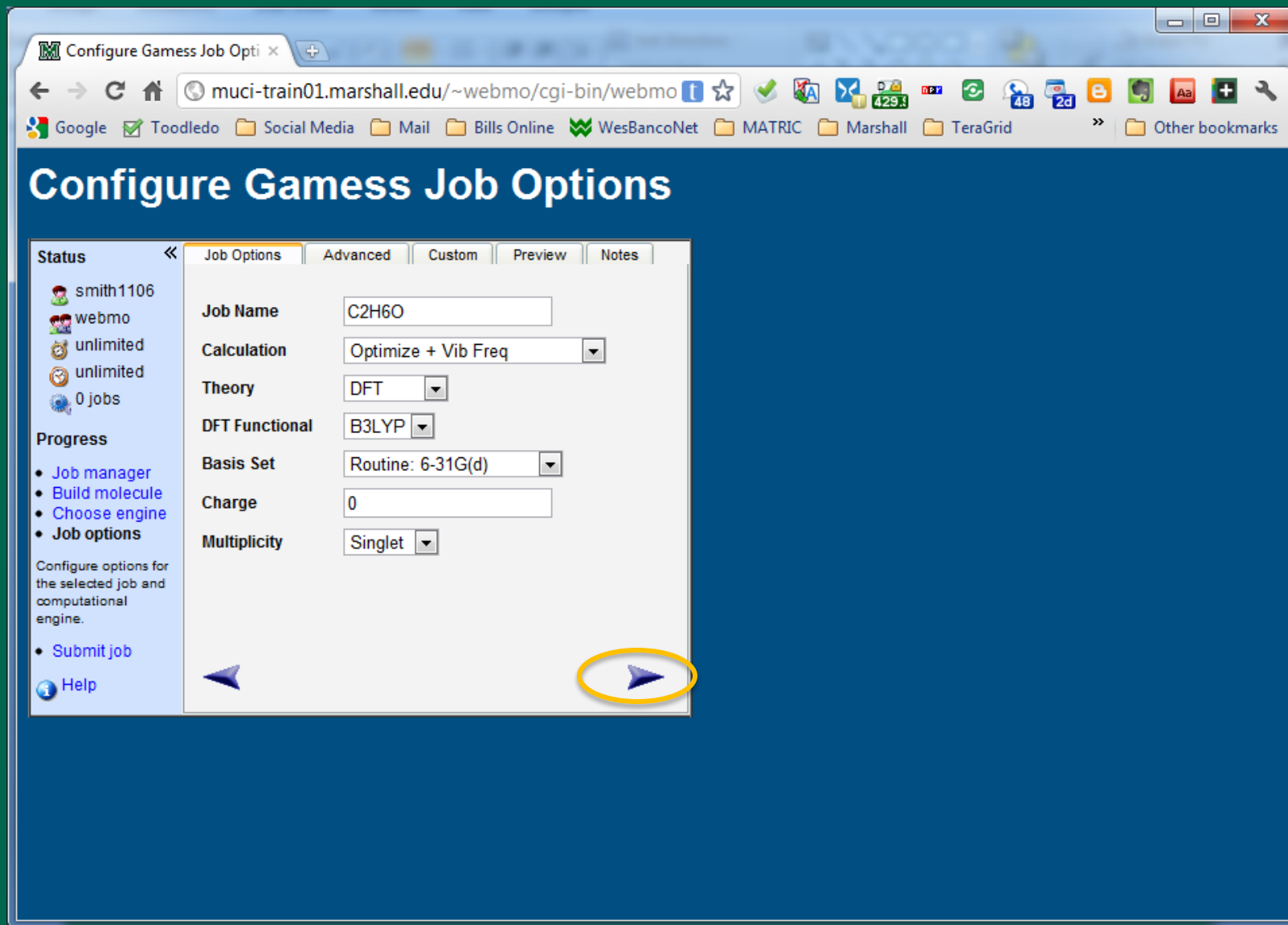
Engine	Description
<input checked="" type="radio"/> Gamess	Ab initio and semi-empirical calculations
<input type="radio"/> Mopac	Semi-empirical calculations
<input type="radio"/> NWChem	Ab initio calculations
<input type="radio"/> Tinker	Molecular mechanics calculations

Select Queue: default

Choose the desired computational engine from those installed.

Submitting Jobs

Configure Job Options

A screenshot of a web browser window showing the 'Configure Gamess Job Options' interface. The browser's address bar shows the URL 'muci-train01.marshall.edu/~webmo/cgi-bin/webmo'. The page has a blue header with the title 'Configure Gamess Job Options'. On the left, there is a sidebar with a 'Status' section showing user 'smith1106', session 'webmo', and '0 jobs'. Below this is a 'Progress' section with links: 'Job manager', 'Build molecule', 'Choose engine', 'Job options', 'Submit job', and 'Help'. The main content area has tabs for 'Job Options', 'Advanced', 'Custom', 'Preview', and 'Notes'. The 'Job Options' tab is active, displaying fields for 'Job Name' (C2H6O), 'Calculation' (Optimize + Vib Freq), 'Theory' (DFT), 'DFT Functional' (B3LYP), 'Basis Set' (Routine: 6-31G(d)), 'Charge' (0), and 'Multiplicity' (Singlet). At the bottom of this tab, there are two blue arrow buttons: a left-pointing arrow and a right-pointing arrow. The right-pointing arrow is circled in yellow.



Submitting Jobs

Monitor Status

WebMO Job Manager

mu-ci-train01.marshall.edu/~webmo/cgi-bin/webmo

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

WebMO Job Manager

Status

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs

Folders

- Inbox
- For Workshop
- Trash
















Manage folders

Empty trash

Search

Displayed jobs

New Job Refresh Download Move To Delete Utilities Logout

Number	Name	Description	Date	Status	Time	Actions
1539	C2H6O	Optimize + Vib Freq - Gamess	8/10/2011 8:36	Running	0.0 sec	  
1516	Vinyl Alcohol	Coordinate Scan - Mopac	8/8/2011 10:17	Complete	2.8 sec	
1515	Vinyl Alcohol	Coordinate Scan - Mopac	8/8/2011 10:13	Complete	4.9 sec	
1509	Acetaldehyde	Vibrational Frequencies - Mopac	8/7/2011 18:19	Complete	0.1 sec	
1508	Acetaldehyde	IRC Calculation (Reverse) - Mopac	8/7/2011 18:15	Complete	0.8 sec	
1507	Acetaldehyde	IRC Calculation (Forward) - Mopac	8/7/2011 18:12	Complete	0.8 sec	
1506	Acetaldehyde	Transition State Optimization - Mopac	8/7/2011 18:11	Complete	0.0 sec	
1505	Acetaldehyde	Saddle Calculation - Mopac	8/7/2011 18:09	Complete	0.5 sec	
1504	Vinyl Alcohol	Geometry Optimization - Mopac	8/7/2011 18:06	Complete	0.0 sec	
1503	Acetaldehyde	Geometry Optimization - Mopac	8/7/2011 18:03	Complete	0.1 sec	
1487	C2HO2F3	Thermochemistry - Mopac	8/6/2011 18:47	Complete	0.5 sec	
1486	C2HO2F3	Geometry Optimization - Mopac	8/6/2011 18:46	Complete	0.7 sec	
1485	C2HO2F3	Thermochemistry - Mopac	8/6/2011 18:45	Complete	0.0 sec	



Viewing Results

- Molecular Viewer
 - Final structure
 - View properties
 - Partial charges, dipole moment
 - Animation
 - Geometry optimization, vibrational modes
 - Input for next job
- Data Viewer
 - Linear plots
 - Spectra (IR, UV-Vis, NMR)
 - 2D maps
- MO Viewer (tabbed)
 - Isosurfaces of MO's and density
 - Texturing with other properties
 - Electrostatic potential
 - Frontier density (electrophilic, nucleophilic and radical susceptibilities)

Viewing Results Molecular Viewer

WebMO Job Manager x 1539 - View Job

muci-train01.marshall.edu/~webmo/cgi-bin/webmo

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

View Job 1539: C2H6O, Optimize + Vib Freq - Gamess

Status

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs

Summary

- C2H6O
- Job # 1539
- 8/10/2011
- 127.5 sec


Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer Data Viewer MO Viewer

File Edit View Help



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

Reset View New Job Using This Geometry Export Molecule



Viewing Results

Calculated Quantities

WebMO Job Manager 1539 - View Job

muci-train01.marshall.edu/~webmo/cgi-bin/webmo

R-B3LYP Energy -154.9387614530 Hartree

Rotational Constants

Constant	Frequency (GHz)	Frequency (cm ⁻¹)
a	34.27356	1.14324290306
b	9.12332	0.30432119810
c	8.06728	0.26909549539

Dipole Moment 1.674433 Debye

Partial Charges

Atom	Symbol	Charge
1	C	-0.456042
2	C	-0.025012
3	O	-0.609141
4	H	0.384251
5	H	0.119577
6	H	0.148583
7	H	0.142930
8	H	0.135027
9	H	0.159827

Bond Order

Atom	Symbol	1 C	2 C	3 O	4 H	5 H	6 H	7 H	8 H	9 H
1	C	-								
2	C	1.006	-							

Viewing Results

Partial Charges

WebMO Job Manager 1539 - View Job

mu-ci-train01.marshall.edu/~webmo/cgi-bin/webmo

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

View Job 1539: C2H6O, Optimize + Vib Freq - Gamess

Status

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs

Summary

- C2H6O
- Job # 1539
- 8/10/2011
- 127.5 sec

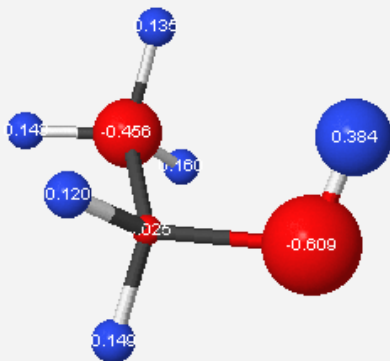
Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer Data Viewer MO Viewer

File Edit View Help



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

Reset Viewer New Job Using This Geometry Export Molecule



Viewing Results

Geometry Optimization

WebMO Job Manager 1539 - View Job

mu-ci-train01.marshall.edu/~webmo/cgi-bin/webmo

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

Calculated Quantities

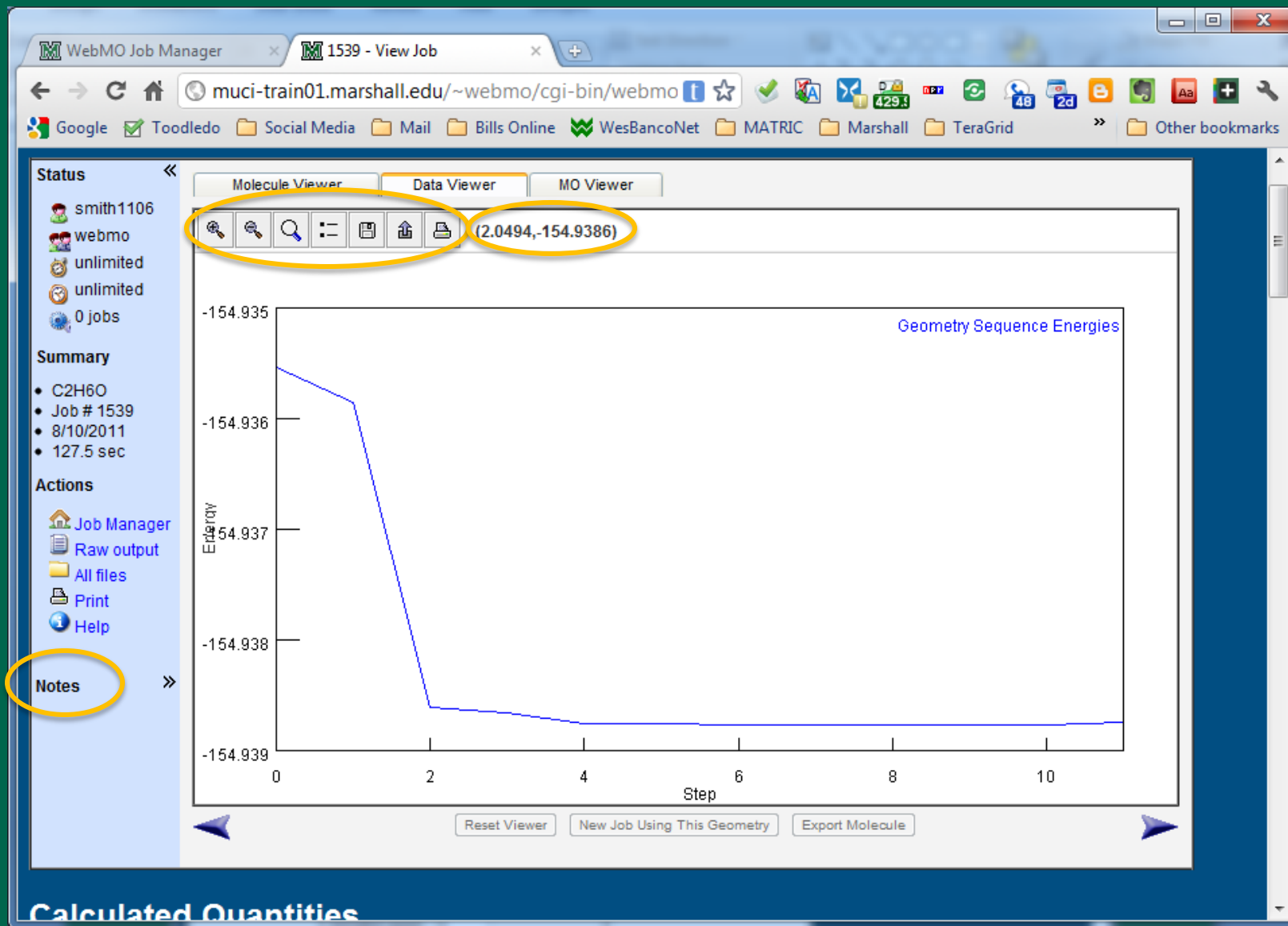
Quantity	Value																										
Route	\$CONTRL SCFTYP= RHF RUNTYP=OPTIMIZE DFTTYP=B3LYP																										
Geometry Sequence	<table><thead><tr><th>Step</th><th>Energy</th></tr></thead><tbody><tr><td>0</td><td>-154.9355339835</td></tr><tr><td>1</td><td>-154.9358533948</td></tr><tr><td>2</td><td>-154.9386092139</td></tr><tr><td>3</td><td>-154.9386580869</td></tr><tr><td>4</td><td>-154.9387547255</td></tr><tr><td>5</td><td>-154.9387573228</td></tr><tr><td>6</td><td>-154.9387729146</td></tr><tr><td>7</td><td>-154.9387733442</td></tr><tr><td>8</td><td>-154.9387738736</td></tr><tr><td>9</td><td>-154.9387739928</td></tr><tr><td>10</td><td>-154.9387740861</td></tr><tr><td>11</td><td>-154.9387484185</td></tr></tbody></table>	Step	Energy	0	-154.9355339835	1	-154.9358533948	2	-154.9386092139	3	-154.9386580869	4	-154.9387547255	5	-154.9387573228	6	-154.9387729146	7	-154.9387733442	8	-154.9387738736	9	-154.9387739928	10	-154.9387740861	11	-154.9387484185
Step	Energy																										
0	-154.9355339835																										
1	-154.9358533948																										
2	-154.9386092139																										
3	-154.9386580869																										
4	-154.9387547255																										
5	-154.9387573228																										
6	-154.9387729146																										
7	-154.9387733442																										
8	-154.9387738736																										
9	-154.9387739928																										
10	-154.9387740861																										
11	-154.9387484185																										

Animation speed

Loop

Viewing Results

Data Viewer



Viewing Results

Molecular Orbitals







































WebMO Job Manager 1539 - View Job

muci-train01.marshall.edu/~webmo/cgi-bin/webmo

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

Molecular Orbitals

Display Range 1 - 16 / 23

Orbital	Symmetry	Occupancy	Energy	Actions
1	A	2	-19.1345 Hartree	 
2	A	2	-10.2247 Hartree	 
3	A	2	-10.1744 Hartree	 
4	A	2	-1.0062 Hartree	 
5	A	2	-0.7396 Hartree	 
6	A	2	-0.6169 Hartree	 
7	A	2	-0.4937 Hartree	 
8	A	2	-0.4438 Hartree	 
9	A	2	-0.4228 Hartree	 
10	A	2	-0.3755 Hartree	 
11	A	2	-0.3642 Hartree	 
12	A	2	-0.3173 Hartree	 
13	A	2	-0.2596 Hartree	 
14	A	0	0.0789 Hartree	 
15	A	0	0.1264 Hartree	 
16	A	0	0.1484 Hartree	 
Electron density				 
Electrostatic potential				 
Electrophilic (HOMO) frontier density				 

HOMO
LUMO

Viewing Results

MO Viewer

WebMO Job Manager x 1539 - View Job

muci-train01.marshall.edu/~webmo/cgi-bin/webmo/

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

Status

smith1106
webmo
unlimited
unlimited
0 jobs

Summary

- C2H6O
- Job # 1539
- 8/10/2011
- 127.5 sec

Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer Data Viewer MO Viewer

File Edit View Help

job1539_mo13 job1539_mo14 job1539_mo13

MO	Occ.	Energy
10	2	-0.3755
11	2	-0.3642
12	2	-0.3173
13	2	-0.2596
14	0	0.0789
15	0	0.1264
16	0	0.1484
17	0	0.1593
18	0	0.1703
19	0	0.1935
20	0	0.2251
21	0	0.2506
22	0	0.5296
23	0	0.5547

Electron density
Electrostatic pot
Elec (HOMO) density
Nuc (LUMO) density
Radical density

Reset Viewer New Job Using This Geometry Export Molecule

Display
Opacity
Slice
Clip
Find
Synchronize Windows
Preferences...

Solid
Transpa
Mesh
Dots

Jmol

Calculated Quantities

Viewing Results

Display Options

WebMO Job Manager 1539 - View Job

mucl-train01.marshall.edu/~webmo/cgi-bin/webmo

View Job 1539: C₂H₆O, Optimize + Vib Freq - Gamess

Status

smith1106
webmo
unlimited
unlimited
0 jobs

Summary

- C₂H₆O
- Job # 1539
- 8/10/2011
- 127.5 sec

Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer Data Viewer MO Viewer

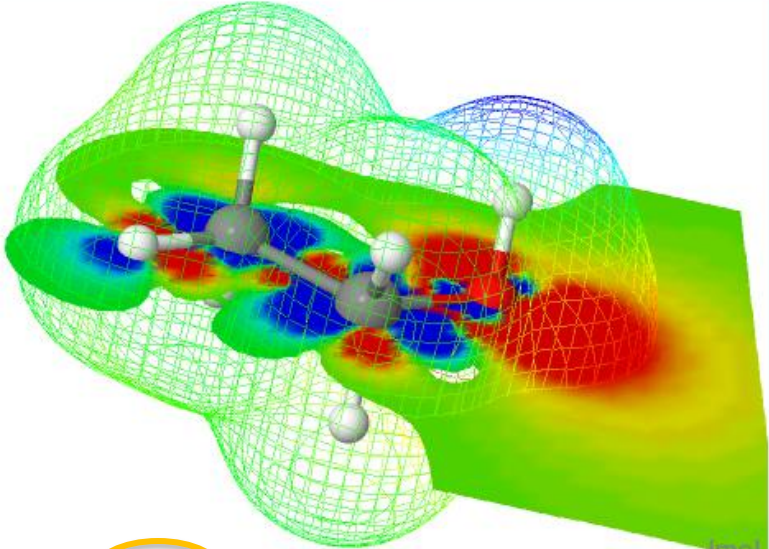
File Edit View Help

job1539_mo13 job1539_mo14 job1539_mo13 job1539_esp

MO	Occ.	Energy
1	2	-19.1345
2	2	-10.2247
3	2	-10.1744
4	2	-1.0062
5	2	-0.7396
6	2	-0.6169
7	2	-0.4937
8	2	-0.4438
9	2	-0.4228
10	2	-0.3755
11	2	-0.3642
12	2	-0.3173
13	2	-0.2596

Electron density
Electrostatic pot
Elec (HOMO) density
Nuc (LUMO) density
Radical density

Reset Viewer New Job Using This Geometry Export Molecule



Viewing Results





















Vibrational Modes



WebMO Job Manager 1539 - View Job


muci-train01.marshall.edu/~webmo/cgi-bin/w

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

Vibrational Modes


Mode	Symmetry	Frequency (cm ⁻¹)	Actions
1	-	258.80	 
2	-	320.57	 
3	-	419.80	 
4	-	809.22	 
5	-	895.82	 
6	-	1070.94	 
7	-	1085.47	 
8	-	1150.36	 
9	-	1296.30	 
10	-	1397.22	 

21 - 3733.08  

Frequency Scale Factor 

Normal Mode Amplitude

Animation Speed

IR Spectrum 

Peak Width (cm⁻¹)

Viewing Results

Animation of Vibrational Mode

WebMO Job Manager 1539 - View Job

mu-ci-train01.marshall.edu/~webmo/cgi-bin/webmo

Google Toodledo Social Media Mail Bills Online WesBancoNet MATRIC Marshall TeraGrid Other bookmarks

View Job 1539: C₂H₆O, Optimize + Vib Freq - Gamess

Status

- smith1106
- webmo
- unlimited
- unlimited
- 0 jobs

Summary

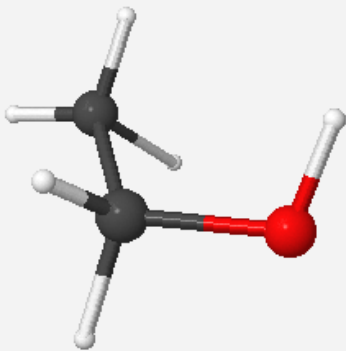
- C₂H₆O
- Job # 1539
- 8/10/2011
- 127.5 sec





Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer Data Viewer MO Viewer



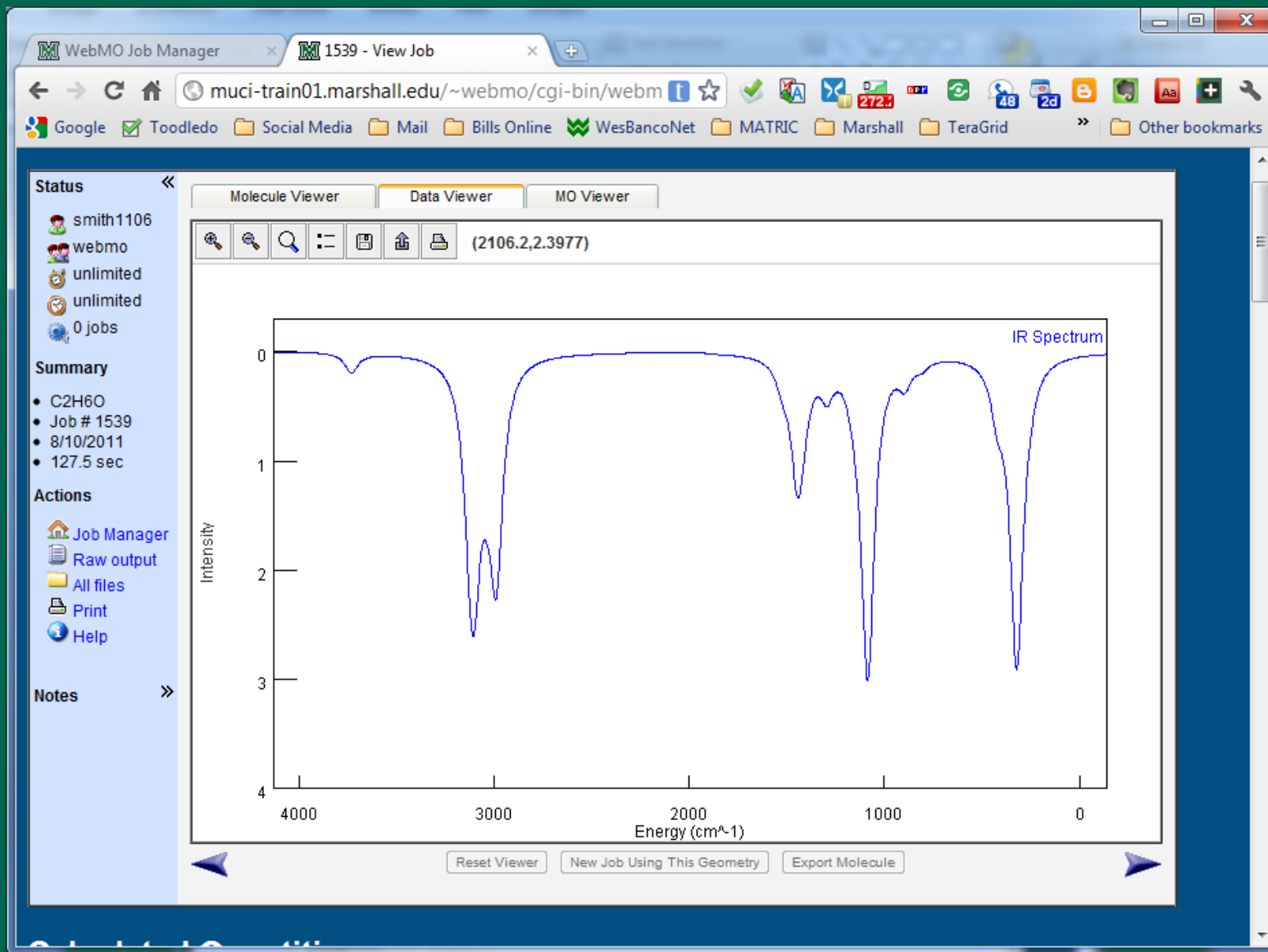





Vibrational mode: ...

[Reset Viewer](#)
[New Job Using This Geometry](#)
[Export Molecule](#)

Viewing Results

IR Spectrum



Viewing Results

Single (UV-Vis) Excitations

WebMO Job Manager x WebMO Job Manager x 1482 - View Job

muci-train01.marshall.edu/~webmo/cgi-bin/webmo

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11	H	0.224300
12	H	0.248339

Excited States

State	Symmetry	Energy (eV)
1	A	4.69
2	A	5.98
3	A	8.55
4	A	8.66
5	A	9.02
6	A	9.27
7	A	9.40
8	A	9.49
9	A	9.87
10	A	9.99

Excitation units: eV

UV-Vis Spectrum

Peak Width (eV): 0.1

Molecular Orbitals

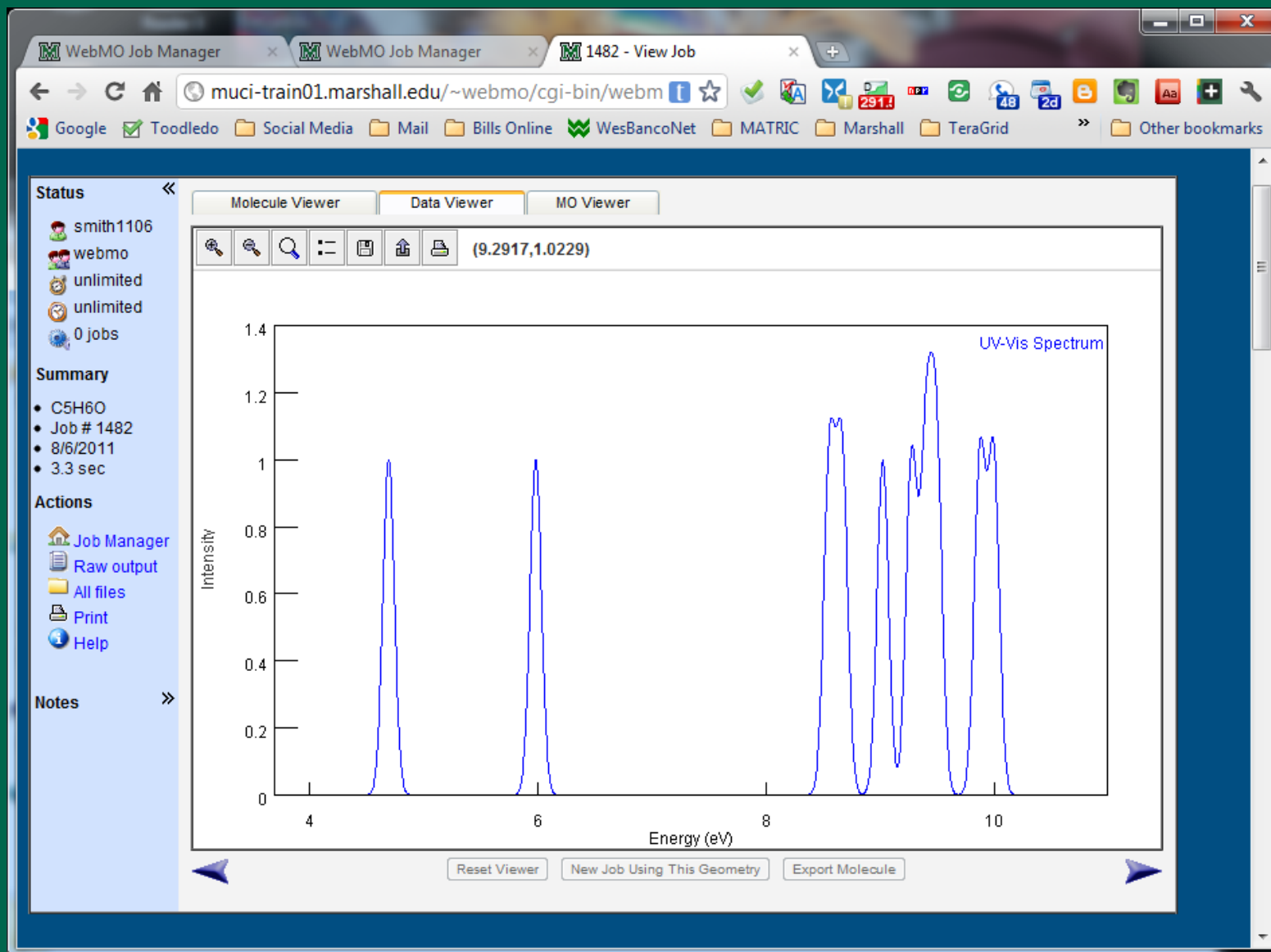
Orbital	Symmetry	Occupancy	Energy	Actions
1	3	2	2 Hartree	

Display Range: 1 - 25 / 60

WineAccess Redux: Having trouble with WineAccess?

Viewing Results

UV-Vis Spectrum



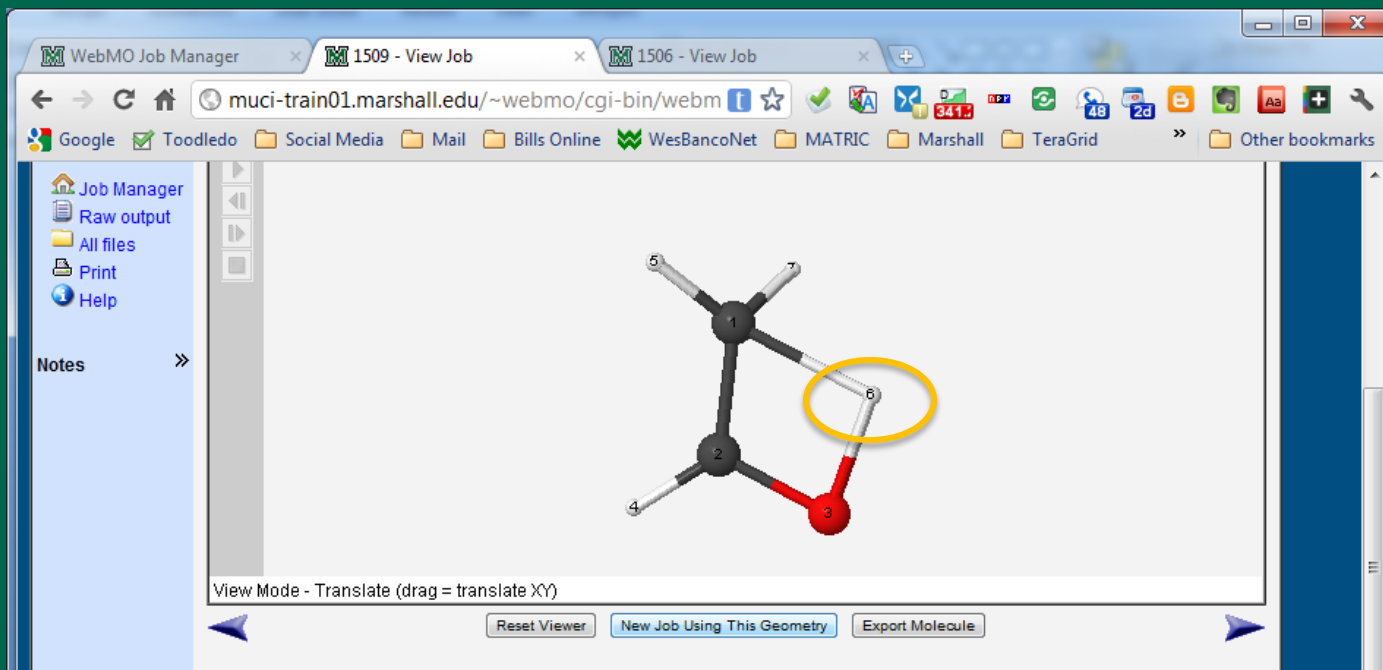


Potential Energy Surface

- Geometry scans (PES)
 - 1 or 2 internal coordinates (distance, angle, dihedral)
- Transition state optimization
 - Saddle point
 - Gradient minimization
 - Confirm one imaginary frequency
- Reaction Coordinate (path)
 - IRC: Intrinsic, kinetic energy dissipated
 - DRC: Dynamic, T+V conserved – *not in WebMO!*







Viewing Results

Transition State



Calculated Quantities

Quantity	Value
Route	
Symmetry	C1
ZPE	31.352 kcal/mol
Vibrational Modes	

Mode	Symmetry	Frequency (cm ⁻¹)	Actions
1	1A	-2569.1	 
2	2A	468.4	 
3	3A	689.7	 

Viewing Results

2-D Geometry Scan

WebMO Job Manager Build Molecule

muci-train01.marshall.edu/~webmo/cgi-bin/webmo

Build Molecule

Status
smith1106
webmo

File Edit Tools View Build Adjust Clean-Up Help

Tools
☒ View
☐ Build
☐ Adjust
☐ Z-Matrix...

Z-Matrix Editor

Order	Atom	Na	Opt	Length	Nb	Opt	Angle	Nc	Opt	Dihedral
1	C1									
2	C2	1	O	1.335						
3	O3	2	O	1.357	1	O	125.508			
4	H4	2	O	1.093	1	O	126.356	3	O	180.000
5	H5	1	O	1.084	2	O	121.566	3	O	180.000
6	H6	1	S	2.500	2	O	50.071	3	S2	0.000
7	H7	1	O	1.086	2	O	124.024	3	O	0.000

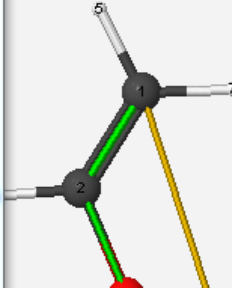
Start Stop # Steps

Scan 2.5 5.0 10

Scan2 0.0 90.0 10

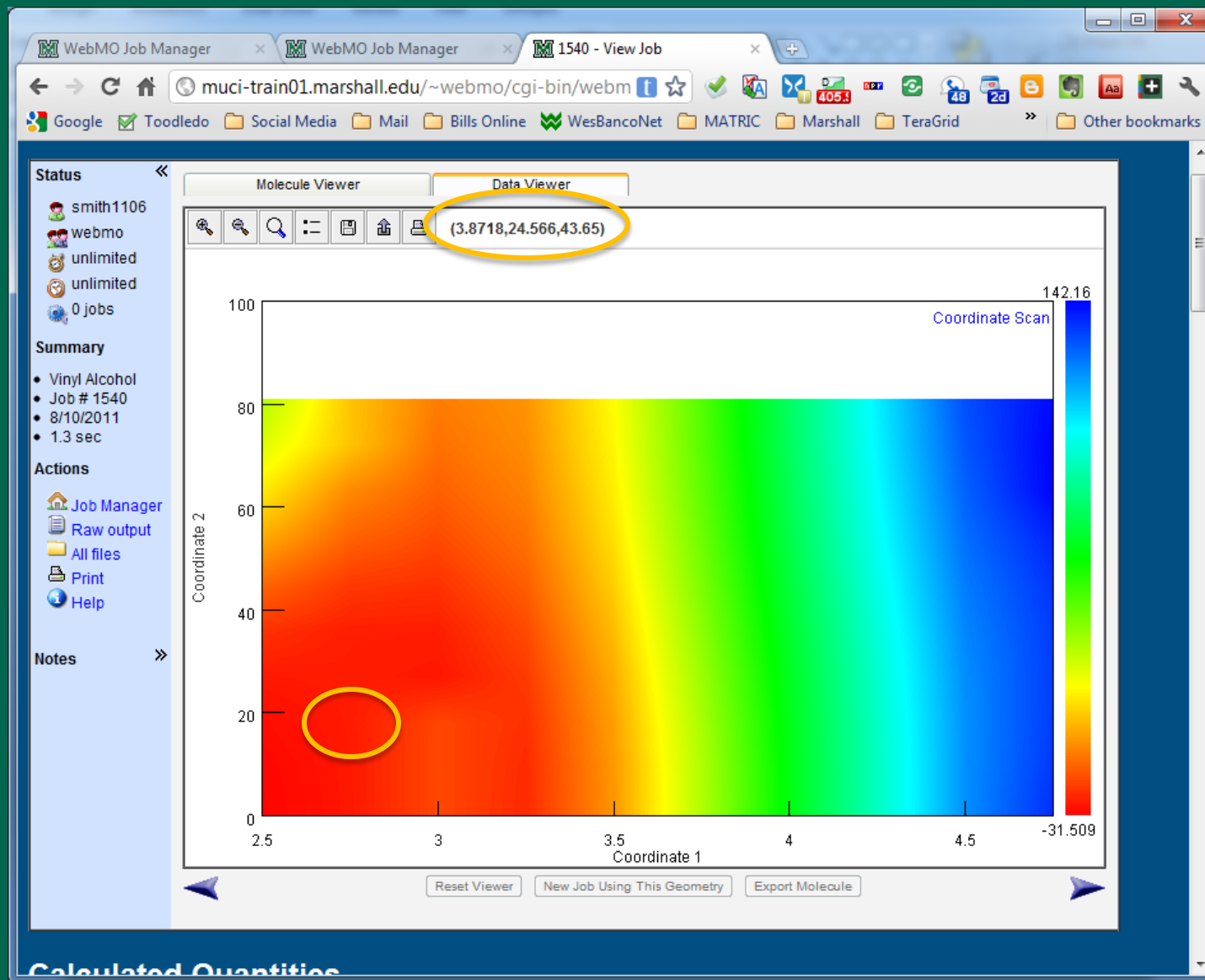
ReOrder ReConnect Opt All Fix All OK

Molecule Export Molecule



Viewing Results

2-D Geometry Scan





Potential Future Topics

- Periodic Systems and Materials Modeling
 - Quantum ESPRESSO, VASP
- Reactivity, QSAR/QSPR
- Spectroscopy and Excited States
- Thermochemistry and Model Chemistries
- Solvation
- Kinetics
- Computational Chemistry – Theory & Practice
- Beyond WebMO
 - Molecular Dynamics
 - Biomolecules (proteins, nucleic acids)
 - Hybrid QM/MM Techniques

Exercise #1

Trifluoroacetic acid (TFA): CF_3COOH

- **Build molecule in 3D editor**
- **Optimize geometry at different levels of theory**
MM3 (Tinker), **PM3 (MOPAC)**, RHF/3-21G, DFT/B3LYP/6-31G(d) (GAMESS)

Visualize optimization

Visualize partial charges (especially acidic H), dipole moment

Visualize orbitals, total and frontier densities, electrostatic potential

Browse output files

- Perform geometry scan of C-C-O-H dihedral
Visualize scan and confirm low-energy conformation

- **Compute and visualize IR spectrum**

Animate vibrational nodes

- Compute deprotonation energy
 $\text{CF}_3\text{COOH} [+ \text{H}_2\text{O}] \rightarrow \text{CF}_3\text{COO}^- [+ \text{H}_3\text{O}^+]$
- Repeat with solvent (H_2O)

Use **MOPAC (PM3)**

Bonus: Compare acidities of $\text{CF}_n\text{H}_{3-n}\text{COOH}$ ($n=0,3$)



Exercise #2

Conjugated aldehyde (enal): $\text{H}_2\text{C}(=\text{CH}-\text{CH})_n=\text{O}$

- **For $n = 1$ (acrolein)**

- Build and optimize structure

- Use MOPAC (PM3)

- Compute and visualize HOMO and LUMO orbitals (and those nearby)

- Use GAMESS: Molecular Orbitals, DFT/B3LYP/6-31G(d)

- Calculate HOMO-LUMO gap (1 hartree = 27.2107 eV) and save

- Compute and visualize UV-Vis (excitation) spectrum

- Use GAMESS: UV-Vis Spectrum, 6-31G(d) -- *ignores level of theory*

- Look at raw output for excitation details (e.g., HOMO \rightarrow LUMO)

- Compare excitation energies with HOMO-LUMO gap

- $1240/\lambda(\text{nm}) = 1 \text{ eV}$

- Repeat above for $n = 2, 3$

- Save results in a spreadsheet and plot HOMO-LUMO gap vs excitation energies

- Save results as HTML (web pages) and view in browser

- **Compare with experiment: 209, 221, 251 (nm)**

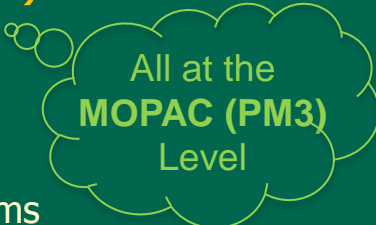
Bonus: Predict and test results for $n > 3$

Exercise #3

Keto-enol tautomerization (proton migration)



- Build and optimize acetaldehyde structure
- Convert acetaldehyde to vinyl alcohol
 - Adding, deleting, and changing bonds only – no adding/deleting atoms
 - Clean hybridization and geometry only – do not add Hydrogens
- Optimize vinyl alcohol structure
 - Remember job#
- Return to acetaldehyde structure and compute the Saddle Point
 - Use job# of vinyl alcohol results as second geometry
- Edit such that H-O-C-C forms a 4-membered ring of single bonds
- Optimize as a Transition State (TS)
- Compute vibrational frequencies
 - Look for one negative (imaginary) frequency and animate it
- Compute IRCs from the TS to both acetaldehyde and vinyl alcohol

A thought bubble with a green outline and three small circles leading to it from the left. Inside the bubble, the text 'All at the MOPAC (PM3) Level' is written in a green, sans-serif font.

All at the
MOPAC (PM3)
Level