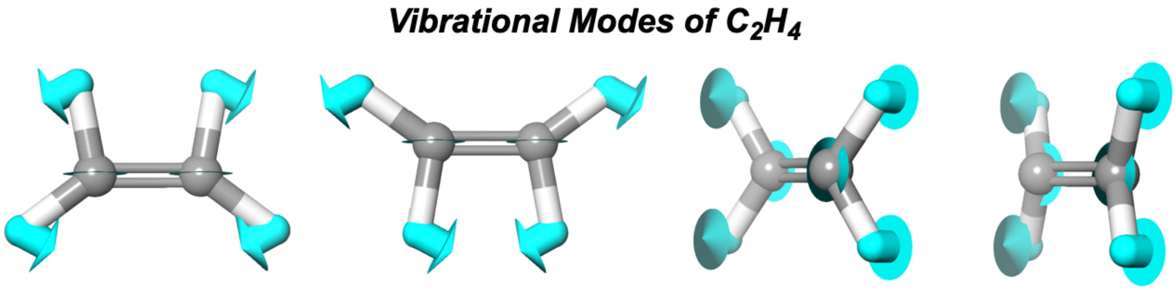
Infrared Spectroscopy



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Infrared Spectroscopy

About this Lesson:

In this lesson, students will learn the fundamentals of infrared (IR) spectroscopy and the many different kinds of vibrational excitation, including stretching and bending. IR spectroscopy can be used to identify which functional groups are present in a compound.

Using Maestro, students will perform frequency calculations and visualize various vibrational modes of small molecules. Students will then generate IR spectra, identify various regions that correspond to particular functional groups, and determine which IR spectrum matches to a given organic compound.

Learning Objectives:

- Explain what IR spectroscopy is and why it is used
- Visualize vibrational modes of small molecules by performing frequency calculations
- Correspond a given IR spectrum to an organic compound through functional group identification

Lesson Contents:

1. Setting Up the Maestro Session
2. Introduction to Infrared spectroscopy
3. Fundamental Vibrational Modes of Water
4. IR-active versus IR-inactive
5. Functional Groups and Trends
6. Resonance Effects
7. Mass Effects
8. Individual Exercises
9. Summary, Additional Resources, and References
10. Glossary of Terms

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Standards Alignment:

- IB Diploma Programme:
    - Models and Representations (Skill 1)
- ACS Guidelines
    - Deducing structures by interpretation of modern spectroscopic and computational data (Practical Topics)
- AAMC MCAT
    - Molecular Structure and Absorption Spectra (4D)

Assessments for Understanding:

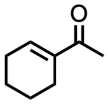
The following types of formative assessments are embedded in this lesson:

- Assessment of student understanding through discussion of warm-up questions and filling in any knowledge gaps about functional group identification
- Visual assessment of student-generated IR spectra and correct molecule matching

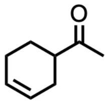
Associated Documentation Pages: Jaguar Geometry Optimization: The Basics

Warm-Up Questions:

Watch the Khan Academy videos on IR spectroscopy.



A



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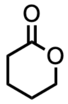
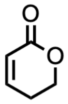


C



D

All of the molecules shown above absorb IR radiation in the range between 1600 and 1850 cm^{-1}. In each molecule:

1) Label the functional groups that are present.

2) Identify the specific bond(s) responsible for the absorption(s) and predict the approximate wavenumber of absorption for each of these bonds.

Need help? Contact us at teaching@schrodinger.com

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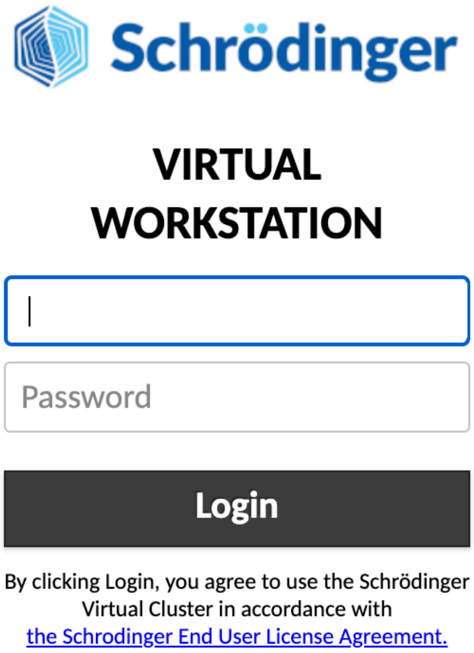
1. Setting Up the Maestro Session

At the start of the Maestro session, it is essential to 1) check your mouse actions, 2) change the file path to the Working Directory for this lesson, and 3) save your project file. The working directory indicated in this section contains the files necessary to complete this lesson. If you do not set the appropriate working directory, you will be unable to run any calculations.

1. Launch the Virtual Cluster



By clicking Login, you agree to use the Schrödinger Virtual Cluster in accordance with the Schrodinger End User License Agreement.

Figure 1-1. Virtual workstation login page.

2. Double-click the **course-data** folder on the desktop

Figure 1-2. Course-data folder on the desktop.

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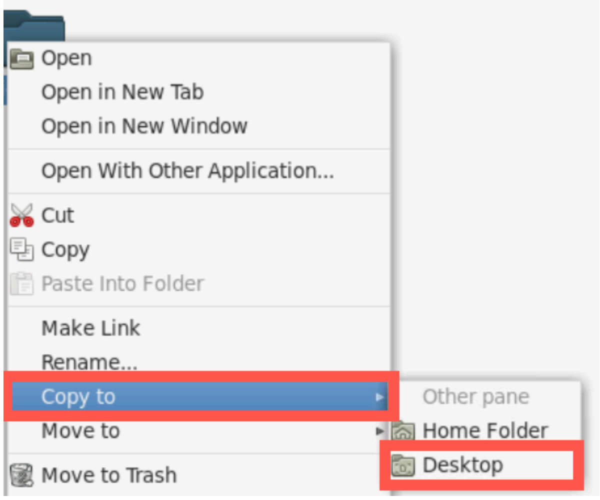
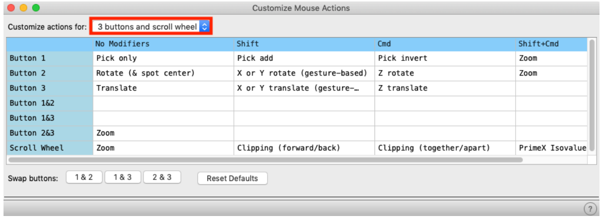


Figure 1-3. Copy the lesson folder to the Desktop.

3. Right-click the `IR_Spectroscopy` folder and select **Copy to > Desktop**

4. Double-click the Maestro icon on the desktop



Customize actions for: 3 buttons and scroll wheel

	No Modifiers	Shift	Cmd	Shift+Cmd
Button 1	Pick only	Pick add	Pick invert	Zoom
Button 2	Rotate (& spot center)	X or Y rotate (gesture-based)	Z rotate	Zoom
Button 3	Translate	X or Y translate (gesture-…	Z translate	
Button 1&2				
Button 1&3				
Button 2&3	Zoom			
Scroll Wheel	Zoom	Clipping (forward/back)	Clipping (together/apart)	PrimeX Isovalue

Figure 1-4. Change the mouse actions.

5. Check your mouse actions.
    - Go to **Workspace > Customize Mouse Actions**
    - *Note:* This lesson was made with a three-button mouse with a scroll wheel, but a trackpad can still be used
    - ***Trackpad keys:***
        - **Up/Down trackpad** = Zoom In/Out
        - **Option** = Rotate
        - **Control** = Translate

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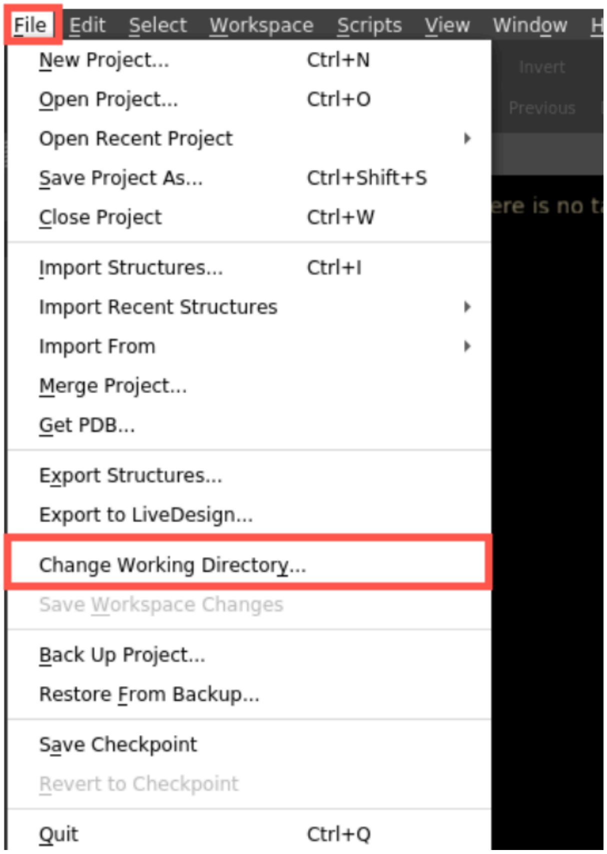
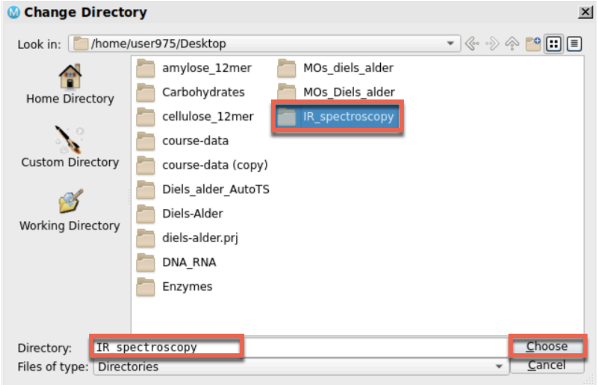


Figure 1-5. Change Working Directory option.

6. Go to File > Change Working Directory



Look in: /home/user975/Desktop

Directory: IR_spectroscopy

Files of type: Directories

Figure 1-6. Change Working Directory panel.

7. Navigate to Desktop > `IR_spectroscopy` folder and click **Choose**

Pre-generated input and results files are included for running jobs or examining output

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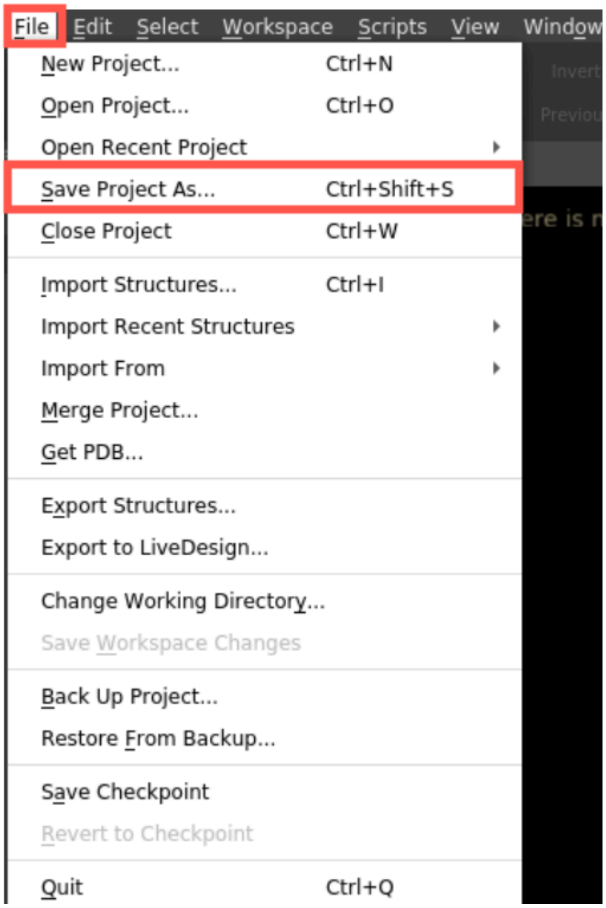
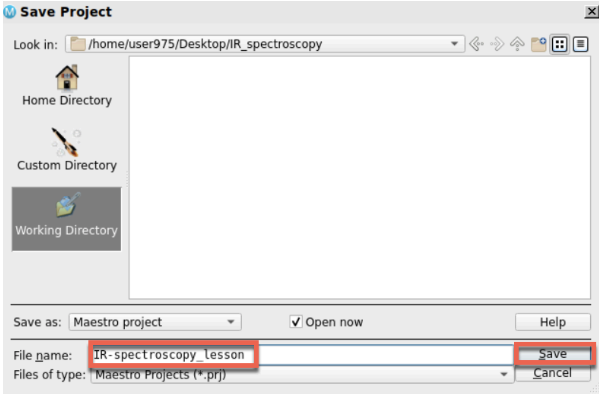


Figure 1-7. Save Project option.

8. Go to File > Save Project As



Look in: /home/user975/Desktop/IR_spectroscopy

Save as: Maestro project

☑ Open now

File name: IR-spectroscopy_lesson

Files of type: Maestro Projects (*.prj)

Figure 1-8. Save Project panel.

9. Change the *File name* to `IR_spectroscopy_lesson`, click Save
    - The project is now named IR_sepctroscopy_lesson.prj

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2. Introduction to Infrared Spectroscopy

Each form of spectroscopy uses a different region of the **electromagnetic spectrum** and involves a different kind of excitation. The interaction between molecules and infrared (IR) radiation promotes **vibrational excitations** of the bonds in a molecule. Each type of bond in a molecule will absorb a characteristic frequency, allowing us to determine which types of bonds are present in a molecule. Chemists irradiate an unknown compound with all frequencies of IR radiation and then detect which frequencies were absorbed. A plot is then constructed showing which frequencies were absorbed by a sample. In this way, **IR spectroscopy** can be used to identify the presence of functional groups in a molecule. IR spectroscopy is commonly used by organic chemists to verify the structures of compounds that are made in a laboratory.

An **IR spectrometer** measures the percent transmittance as a function of frequency. A plot called an absorption spectrum is generated where each signal, called an absorption band, points downwards on an IR spectrum. The position where a signal lies corresponds to a frequency-related unit called a **wavenumber** in units of inverse centimeters (cm^{-1}) where the values can range from 400 to 4000 cm^{-1}. It's important to note that wavenumber is proportional to frequency; therefore, a larger wavenumber represents higher energy. Signals that appear on the left side of an IR spectrum correspond with higher energy radiation, whereas signals on the right side of an IR spectrum correspond with lower energy radiation.

There are three characteristics in every signal that appears in an IR spectrum: wavenumber, intensity, and shape. The wavenumber of a signal is determined by bond strength and the masses of the atoms sharing the bond. The **intensity** of a signal is dependent on the dipole moment of the bond giving rise to the signal. The **shape** of a signal can either be broad or sharp. Each type of functional group lies within a certain region of an absorption spectrum. Use the IR spectroscopy functional group stretching frequency chart that your instructor has provided you.

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3. Fundamental Vibrational Modes of Water

IR radiation causes vibrational excitation of the bonds in a molecule. There are different kinds of vibrational excitation since bonds store vibrational energy in a number of ways. Bonds can **stretch**, similar to how a spring stretches, and bonds can also **bend** in various directions. Even though there are several types of bending vibrations, we will mostly be focusing on various stretching vibrations.

In this section, we will learn the steps for performing a standard frequency calculation. We will also analyze the vibrational modes of a water molecule and view the predicted spectrum.

Computational Exercise #1: Analyzing the vibrational modes of water

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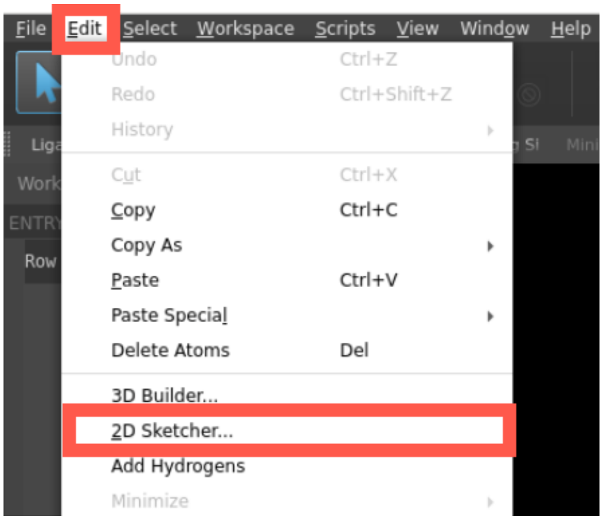

Figure 3-1. Open 2D Sketcher.

1. Go to **Edit > 2D Sketcher**
2. **Draw** the structure of H_2O
3. Click on **Save as New** and for *Input Entry Title* write **water**. Click **OK**.

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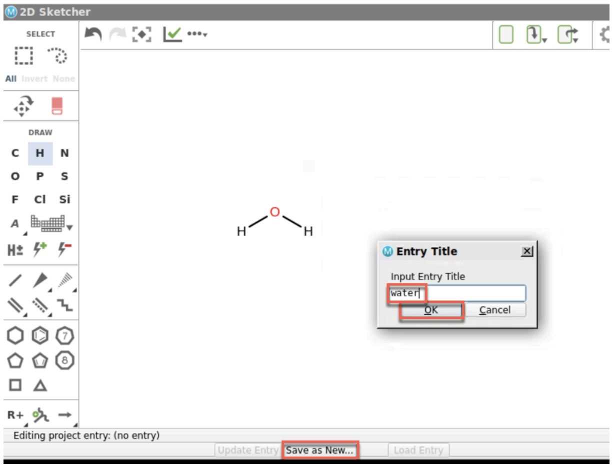

Input Entry Title: water

Editing project entry: (no entry)

Figure 3-2. Sketching and saving H_2O.

The 2D sketcher functions like many standard 2D molecular drawing tools. For a complete overview of using the sketcher panel, see the 2D Sketcher Panel documentation.

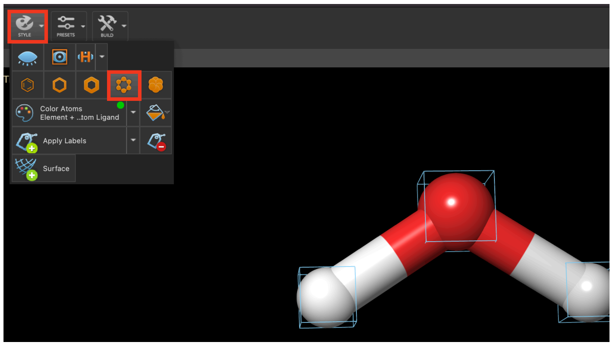

Figure 3-3. Viewing and stylizing H_2O.

4. Close the 2D Sketcher panel
    a. The H_2O molecule is selected in the entry list and included in the workspace
5. Change the representation to the ball-and-stick by clicking on the **Style** menu and choosing **Apply ball-and-stick representation**

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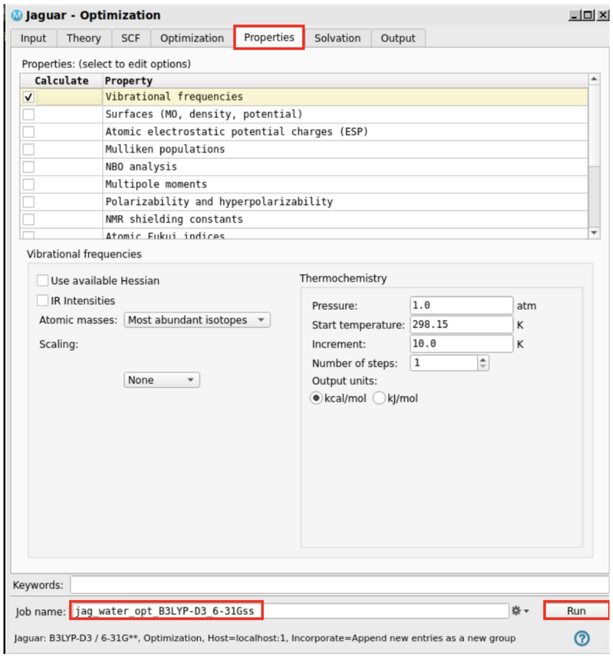


Properties: (select to edit options)

Calculate	Property
☑	Vibrational frequencies
☐	Surfaces (MO, density, potential)
☐	Atomic electrostatic potential charges (ESP)
☐	Mulliken populations
☐	NBO analysis
☐	Multipole moments
☐	Polarizability and hyperpolarizability
☐	NMR shielding constants
☐	Atomic Fukui indices

Vibrational frequencies

☐ Use available Hessian
☐ IR Intensities
Atomic masses: Most abundant isotopes
Scaling: None

Thermochemistry

Pressure: 1.0 atm
Start temperature: 298.15 K
Increment: 10.0 K
Number of steps: 1
Output units: ● kcal/mol ○ kJ/mol

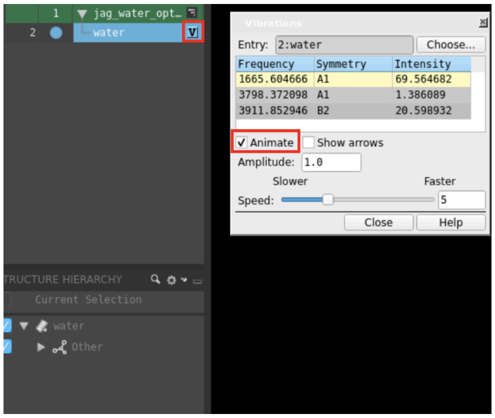
Keywords:
Job name: jag_water_opt_B3LYP-D3_6-31Gss

Jaguar: B3LYP-D3 / 6-31G**, Optimization, Host=localhost:1, Incorporate=Append new entries as a new group

Figure 3-4. Setting the Optimization panel.

Now let us optimize the molecule at the quantum mechanical level and request a frequency calculation.

6. With the H2O entry selected and included, go to **Tasks > Jaguar > Optimization**
    a. The Jaguar - Optimization panel opens
7. Maintain the defaults on the *Input* tab
8. On the *Properties* tab, check **Calculate** for **Vibrational frequencies**
9. **Run** the job



Entry: 2:water

Frequency	Symmetry	Intensity
1665.604666	A1	69.564682
3798.372098	A1	1.386089
3911.852946	B2	20.598932

☑ Animate ☐ Show arrows
Amplitude: 1.0
Slower Faster
Speed: 5

Figure 3-5. Animating the vibrations.

When the job completes, an output group is incorporated into the entry list

10. Select and include the output entry
11. Click the vibration viewer button V

Three frequencies are shown as well as the symmetry and intensity

12. **Check** Animate and visualize all three modes (bending, symmetric stretching and antisymmetric stretching)

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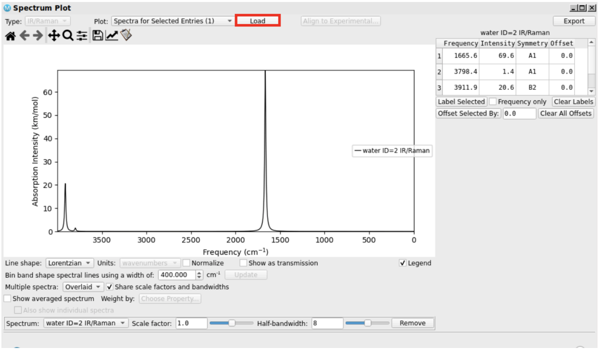
Pause & Think #1. Take screenshots of all three vibrational modes of water:

Bending	Symmetric Stretching	Antisymmetric Stretching



Type: IR/Raman Plot: Spectra for Selected Entries (1)

water ID=2 IR/Raman

	Frequency	Intensity	Symmetry	Offset
1	1665.6	69.6	A1	0.0
2	3798.4	1.4	A1	0.0
3	3911.9	20.6	B2	0.0

☐ Frequency only

Offset Selected By: 0.0

Line shape: Lorentzian Units: wavenumbers ☐ Normalize ☐ Show as transmission ☑ Legend

Bin band shape spectral lines using a width of: 400.000 cm⁻¹

Multiple spectra: Overlaid ☑ Share scale factors and bandwidths

☐ Show averaged spectrum Weight by: Choose Property...

☐ Also show individual spectra

Spectrum: water ID=2 IR/Raman Scale factor: 1.0 Half-bandwidth: 8

Figure 3-6. Plotting the IR spectrum.

You can plot the spectrum.

13. With the output entry selected and included, go to **Tasks > Jaguar > Plot Spectra**
    a. The Spectrum Plot panel opens
14. Click **Load**

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Pause & Think #2. The predicted gas phase IR spectrum is shown. Take a screenshot of the IR spectrum for the IR worksheet.

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4. IR-active versus IR-inactive

In this section, we will study the frequency output for acetylene to visualize the difference between IR-active and IR-inactive modes.

Computational Exercise #2: Visualizing IR-active versus IR-inactive modes

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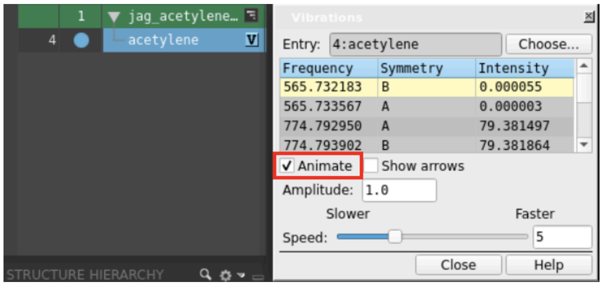

Entry: 4:acetylene

Frequency	Symmetry	Intensity
565.732183	B	0.000055
565.733567	A	0.000003
774.792950	A	79.381497
774.793902	B	79.381864

☑ Animate ☐ Show arrows

Amplitude: 1.0

Speed: 5

Figure 4-1. Animating the vibrations for C_2H_2.

1. Repeat the above steps performed for H_2O for an **acetylene** molecule (C_2H_2)
    - ○ Sketch, save, visualize and perform QM calculation
2. Select and include the output entry
3. Click the vibration viewer button V

Seven frequencies are shown as well as the symmetry and intensity

4. **Check** Animate and visualize all seven modes .

Pause & Think #3. Take screenshots of all seven vibrational modes of acetylene:

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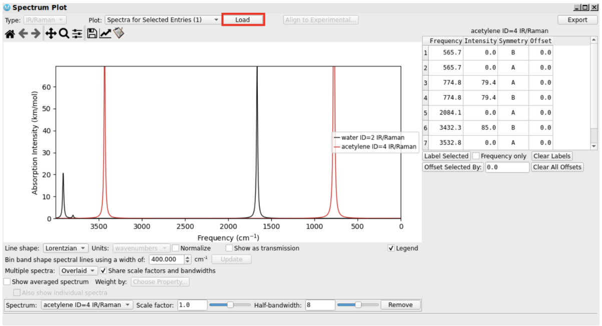
Vibrations of bonds with dipole moments generally result in IR absorptions that are ‘active,’ whereas modes in which the vibration produces no change in the dipole moment are typically ‘inactive.’



Type: IR/Raman

Plot: Spectra for Selected Entries (1)

acetylene ID=4 IR/Raman

	Frequency	Intensity	Symmetry	Offset
1	565.7	0.0	B	0.0
2	565.7	0.0	A	0.0
3	774.8	79.4	A	0.0
4	774.8	79.4	B	0.0
5	2084.1	0.0	A	0.0
6	3432.3	85.0	B	0.0
7	3532.8	0.0	A	0.0

☐ Frequency only

Offset Selected By: 0.0

Line shape: Lorentzian

Units: wavenumbers

☐ Normalize

☐ Show as transmission

☑ Legend

Bin band shape spectral lines using a width of: 400.000 cm^{-1}

Multiple spectra: Overlaid

☑ Share scale factors and bandwidths

☐ Show averaged spectrum

Weight by: Choose Property...

☐ Also show individual spectra

Spectrum: acetylene ID=4 IR/Raman

Scale factor: 1.0

Half-bandwidth: 8

Figure 4-2. Predicted acetylene IR spectrum.

5. Plot the IR spectrum following the same steps from **Section 2**, take a screenshot, and put it in the IR worksheet. Notice that only two peaks appear.

Pause & Think #4. Take a screenshot of the predicted gas phase IR spectrum of acetylene

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5. Functional Groups and Trends

In this section, we will study the frequency output for several organic molecules to familiarize ourselves with the typical shifts associated with different functional groups.

<u>Computational Exercise #3:</u> Frequency output for different functional groups

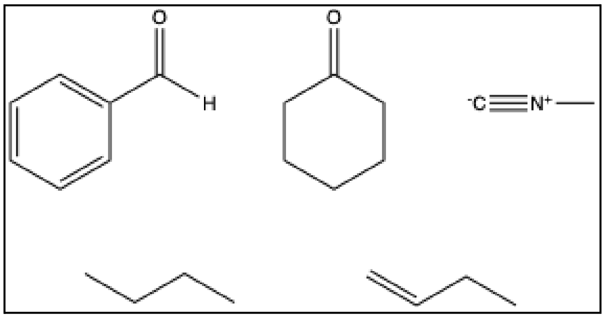

Figure 5-1. Structures to draw.

1. Repeat the above steps performed for H_2O for the organic molecules shown in Figure 3-1
    - Sketch, save, visualize and perform QM calculation

Note: Recall that these jobs can be submitted and run simultaneously by selecting all of the entries before opening the Jaguar - Optimization panel

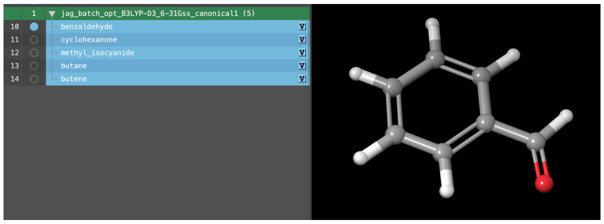

Figure 5-2. Outputs for five organic molecules.

Proceed to analyze the vibrations for the various organic molecules. Can you identify the diagnostic aldehyde C-H stretch, the carbonyl stretch, the CN triple bond? What are the key differences between the butane and 1-butene spectra?

- Fill in the Table with diagnostic frequencies in the IR worksheet

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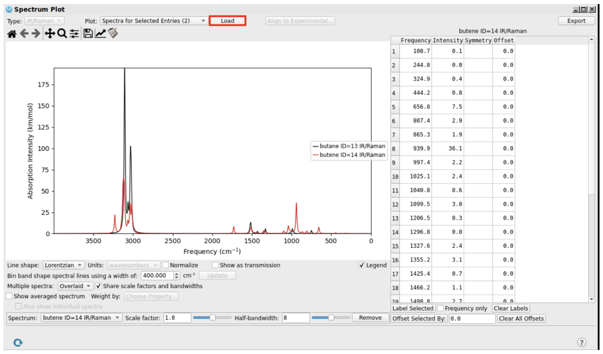

Line shape: Lorentzian   Units: wavenumbers   ☐ Normalize   ☐ Show as transmission   ☑ Legend
Bin band shape spectral lines using a width of: 400.000 cm⁻¹
Multiple spectra: Overlaid   ☑ Share scale factors and bandwidths
☐ Show averaged spectrum   Weight by:
☐ Also show individual spectra
Spectrum: butene ID=14 IR/Raman   Scale factor: 1.0   Half-bandwidth: 8

butene ID=14 IR/Raman

	Frequency	Intensity	Symmetry	Offset
1	108.7	0.1		0.0
2	244.8	0.0		0.0
3	324.9	0.4		0.0
4	444.2	0.8		0.0
5	656.8	7.5		0.0
6	807.4	2.9		0.0
7	865.3	1.9		0.0
8	939.9	36.1		0.0
9	997.4	2.2		0.0
10	1025.1	2.4		0.0
11	1040.8	8.6		0.0
12	1099.5	3.0		0.0
13	1206.5	0.3		0.0
14	1296.8	0.0		0.0
15	1327.6	2.4		0.0
16	1355.2	3.1		0.0
17	1425.4	0.7		0.0
18	1466.2	1.1		0.0
19	1498.8	2.7		0.0

☐ Frequency only
Offset Selected By: 0.0

Figure 5-3. Outputs for five organic molecules.

To answer the latter question, let's overlay the spectra from butane and 1-butene in the spectra viewer.

2. **Select** both the output from butane and butene
3. Go to **Tasks > Jaguar > Plot Spectra**
    - ○ The Spectrum Plot panel opens
4. Click **Load**
5. **Normalize** the spectra
6. View in either **Stacked** mode or **Overlaid**

There are two noticeable characteristics that differentiate the butane and 1-butene spectra

6. Resonance Effects

In this section, we will compare the IR frequency output for cyclohexanone and 2-cyclohexen-1-one to demonstrate the effect of resonance on diagnostic modes.

<u>Computational Exercise #4:</u> Frequency output for cyclohexanone and 2-cyclohexen-1-one

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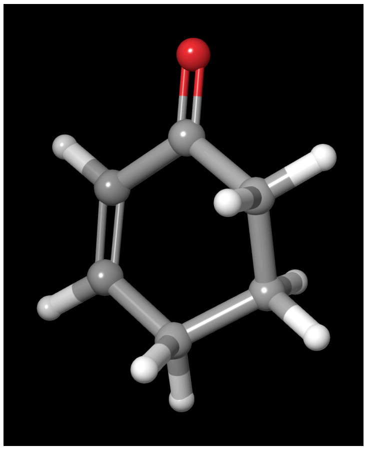


Figure 6-1. 2-cyclohexen-1-one in the workspace.

1. Repeat the above steps performed for 2-cyclohexen-1-one
    - ○ Sketch, save, visualize and perform QM calculation

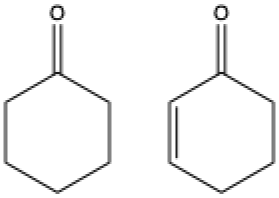
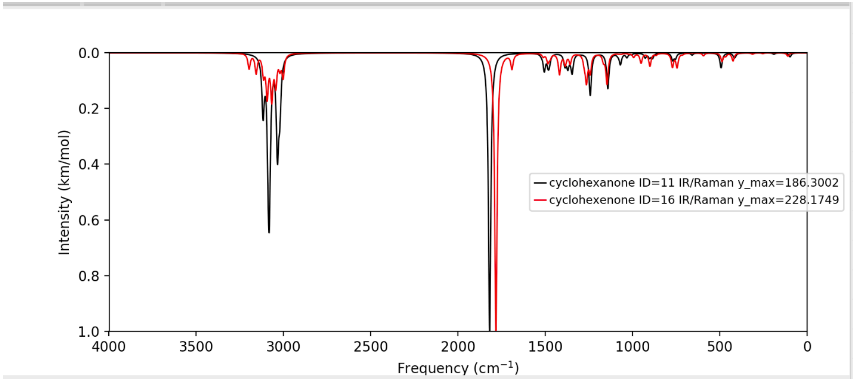


Figure 6-2. Structures.

Compare the key carbonyl vibrations for the two compounds. Which stretching frequency is lower? Can you explain why based on a simple Lewis structure approach? Answer these questions in the IR worksheet.



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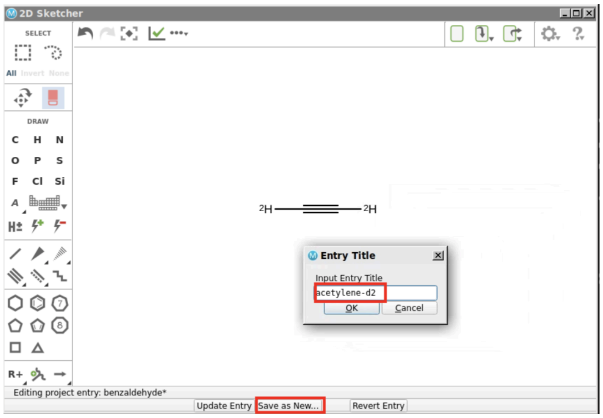
7. Mass Effects

In this section, we will compare the IR frequency output for acetylene and acetylene-d_2 to demonstrate the effect of mass on diagnostic modes.

<u>Computational Exercise #5:</u> Frequency output for acetylene and acetylene-d_2



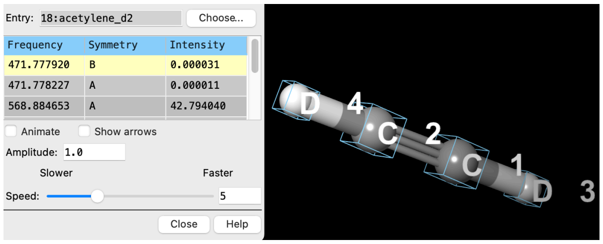
Input Entry Title: acetylene-d2

Editing project entry: benzaldehyde*

Figure 7-1. Adding deuterium to the acetylene model.

1. Repeat the above steps for acetylene-d_2
    - ○ Sketch, save, visualize and perform QM calculation

Note: In the 2D sketcher, hover over a hydrogen with your mouse and type ‘d’ on your keyboard to change the hydrogen to a deuterium atom. Alternatively, right-click the hydrogens in the workspace and adjust the isotope.



Entry: 18:acetylene_d2

Frequency	Symmetry	Intensity
471.777920	B	0.000031
471.778227	A	0.000011
568.884653	A	42.794040

☐ Animate ☐ Show arrows

Amplitude: 1.0

Slower Faster

Speed: 5

Figure 7-2. Vibrations for the acetylene-d_2 structure.

Compare the IR spectra of acetylene and acetylene-d_2.

What do you notice about the spectrum of the non-deuterated molecule as compared to the deuterated molecule? Why do you think this difference is observed? How can this be useful for a synthetic chemist?

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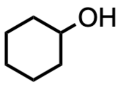
8. Individual Exercises

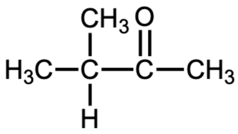
Two infrared spectra are shown, corresponding to two of the following compounds. Match the corresponding structure to each IR spectrum by:

1) Identifying how the major peaks (above 1500 cm^{-1}) in each spectrum correspond to the structure you have chosen
2) Using molecular modeling to perform a vibrational analysis with Maestro to confirm your answers

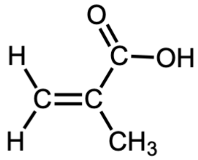
Structure Bank:



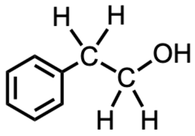
1



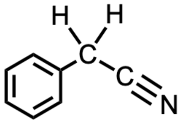
2



3

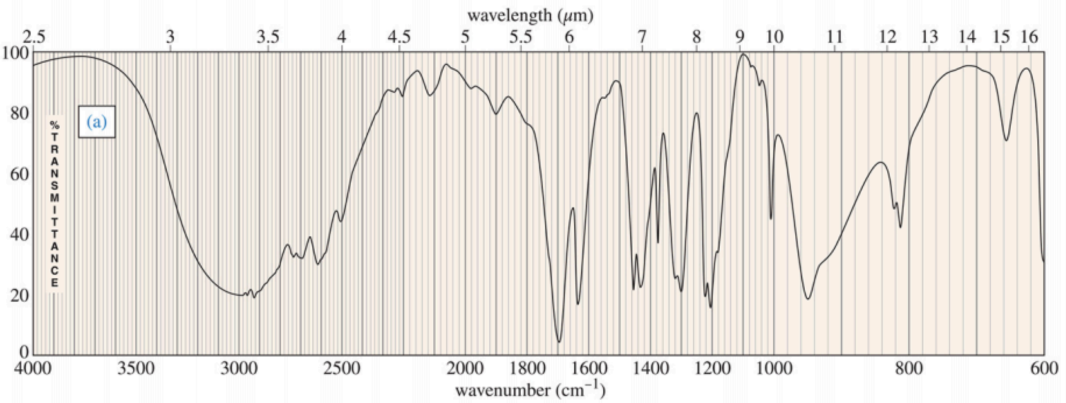


4



5

IR Spectrum A:



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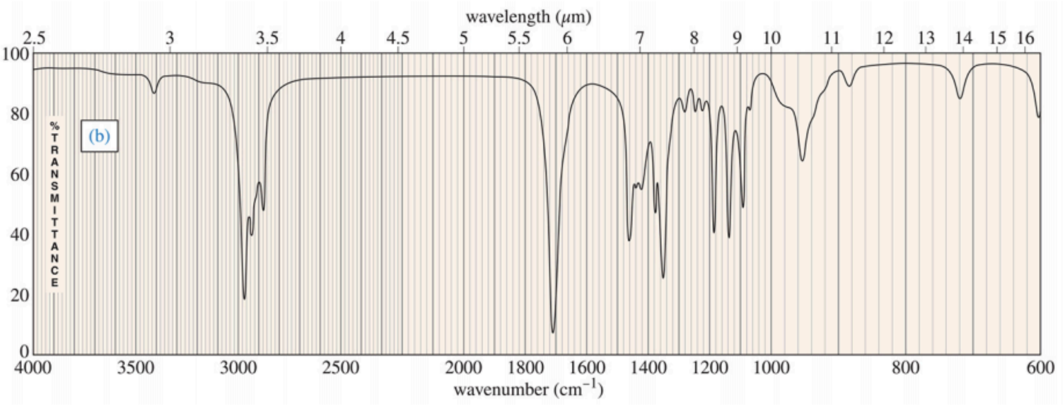
IR Spectrum B:



9. Summary, Additional Resources, and References

For further learning:

For introductory content, focused on navigating the Schrödinger Materials Science interface, Getting Started with Schrödinger for Materials Science is available.

For some related practice, proceed to explore other relevant tutorials:

- Introduction to Multistage Quantum Mechanical Workflows
- Locating Transition States
- Optoelectronics
- Band Shape
- pKa Predictions with Jaguar pKa
- Computing Atomic Charges with Jaguar

For further reading:

- Introduction to Computational Chemistry, 3rd Edition
- Essentials of Computational Chemistry: Theories and Models, 2nd Edition
- See the Jaguar help documentation

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10. Glossary of Terms

Entry List - a simplified view of the Project Table that allows you to perform basic operations such as selection and inclusion

Included - the entry is represented in the Workspace, the circle in the In column is blue

Project Table - displays the contents of a project and is also an interface for performing operations on selected entries, viewing properties, and organizing structures and data

Recent actions - This is a list of your recent actions, which you can use to reopen a panel, displayed below the Browse row. (Right-click to delete.)

Scratch Project - a temporary project in which work is not saved. Closing a scratch project removes all current work and begins a new scratch project

Selected - (1) the atoms are chosen in the Workspace. These atoms are referred to as "the selection" or "the atom selection". Workspace operations are performed on the selected atoms. (2) The entry is chosen in the Entry List (and Project Table) and the row for the entry is highlighted. Project operations are performed on all selected entries

Working Directory - the location that files are saved

Workspace - the 3D display area in the center of the main window, where molecular structures are displayed

2D Workspace - the 2D panel that opens from the “edit” dropdown that allows for the construction of molecules using a 2D sketcher

Tile - if multiple entries are included, included entries are displayed side by side in individual boxes rather than being overlaid in the same space

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