A COMPUTATIONAL STUDY OF SCN

REPORT INSTRUCTIONS

All work for this experiment must be recorded, attached, or answered in the ELN. Create a pre and inlab page in the Week 3’s folder. An objectives and observations (data) sections are required, chemical/equipment tables and procedures are NOT required. All Spartan or Excel data collected or files created should be recorded or attached in the observations section. Create a postlab page in Week 3’s folder to answer the questions at the end of this document.

INTRODUCTION

Electrons are responsible for most chemical and physical properties. So, to understand molecules and polyatomic ions, we must first understand electrons. What volume of space do they occupy? Where are they most likely to be found? What is their energy? What are orbitals?

When an electric discharge is used to excite a sample of elemental gas like hydrogen or neon, light is emitted. When the light emitted is passed through a prism, it is separated into different colors to reveal specific sharp line (colors) of light (with specific wavelengths). Each element has its own unique set of lines, which together create an emission spectrum. The source of the emission lines is the release of photons of specific energy from atoms in the excited state: an electron is promoted into a higher (excited state) orbital by the electric discharge; when that electron goes back to its original ground state orbital, the energy is released as a photon (Figure 1). Each photon's wavelength (and therefore, energy \( E = h \nu \)) is equal to the difference in energy \( \Delta E = E_{\text{UO}} - E_{\text{OO}} \) of the ground and excited state orbitals.

![Energy Levels Diagram]

\[ \Delta E = h \nu \]

\[ \text{Photon of Colored Light Emitted} \]

\[ E_{\text{LUMO}} \]

\[ E_{\text{HOMO}} \]

\[ E_{\text{LUMO}} \]

\[ E_{\text{HOMO}} \]

Figure 1. Electron return to the ground state results in a line on an emission spectrum.
Early investigators found that the wavelengths for the lines of the hydrogen emission spectra can be calculated with the Rydberg equation:

\[
\frac{1}{\lambda} = R_H \frac{(n_f^2 - n_i^2)}{(n_i - n_f)}
\]

Niels Bohr explained this mathematical regularity by proposing the quantization of atoms. He postulated that electrons moved around the nuclei in fixed orbits. He defined the \(n_l\) (\(n\) for the lower energy state) and the \(n_h\) (\(n\) for the higher energy state) in the Rydberg equation as quantum numbers indicating which orbit an electron was in relative to the nucleus. Bohr's theory only goes so far though, the Rydberg equation only works for hydrogen atoms. However, it was one of the first attempts to describe of an electron's energy and location. You will investigate the Rydberg equation in the Sapling pre-lab homework for this experiment.

After Bohr, electronic theories became increasingly more mathematically complex. The advent of computers in the 1950s enabled scientists to begin to find solutions. Now many computational molecular modeling programs are available. In this course we will use Spartan. (Note: Computational Chemistry is one of the fastest growing fields in chemistry. Many Chemistry Professors here at UC Irvine do research in this field.)

The fundamental theory used in computational chemistry is from Erwin Schrödinger. Schrödinger postulated that the tiny electron, while a particle with mass, also behaves like a wave. He proposed the idea of wave functions (orbitals), a mathematical description of an electron's three-dimensional location in space. Wave functions are incredibly complex formulae, in fact, only the wave function for a neutral hydrogen atom (or a 1 e⁻ ion) can be completely solved. (All other wave functions are approximated/simplified by the use of various assumptions.) Here is the equation for a hydrogen atom:

\[
\psi_{nlm}(r,\theta,\phi) = R_n(r) \cdot Y_{lm}^{\phi}(\theta,\phi)
\]

\[
R_n(r) = -\frac{4(n - l - 1)!^{1/2}}{n^4[(n+1)!]^3} (2r)^l \frac{L^2 r^l}{n^{3/2} (2r)^{n/2}}
\]

\[
Y_{lm}^{\phi}(\theta,\phi) = \frac{[(2l+1)(l - |m_l|)!]^{1/2} P_{|m_l|}^l(\cos\theta) + (2\pi)^{1/2} e^{im_l \phi}}{[2(1 + |m_l|)!]^{1/2}}
\]

The above equations contain quantum numbers (\(n, l\), and \(m\)) that take different values depending on the desired orbital of the 1 e⁻ atom. (For example, if \(n = 1, l = 0, m = 0\), \(\psi_{1s}\) will be calculated; if \(n = 2, l = 1, m = 0\), \(\psi_{2p}\) will be calculated.) Spherical \((r,\theta,\phi)\) (instead of Cartesian \((x,y,z)\)) coordinates are used to describe the motion of the electrons around a center nucleus. The connection between the two types of coordinates is demonstrated below (Figure 2).

Look at the very end of the spherical \((Y_{lm})\) component (the last equation) of \(\psi_{1s}\). Do you see the "i" in the \(e^{im_l \phi}\) term? This complex number \((i = \sqrt{-1})\) is a mathematical indication of phase. What is phase? Waves have phase: if two waves come together in phase (both at the crest or both at
the trough), the wave grows larger; if two waves come together out of phase (one at the crest and one at the trough), the waves are cancelled out. Because an electron is treated as a particle and a wave, an analogy is made likening the two waves coming together to two atomic orbitals coming together to form two molecular orbital.

**Figure 2.** Relationship between Spherical & Cartesian Coordinates.

When two atomic wave functions (\(\psi\), atomic orbitals, AOs) come together in phase a bonding molecular wave function (\(\Psi\), molecular orbital, MO) (a larger wave) is created (Figure 3). However, if the same two AOs come together out of phase an antibonding MO (no wave) is created (Figure 4).

**Figure 3.** In phase overlap of two p AOs (\(\psi_a + \psi_b\)) to create a \(\sigma\) bonding MO (\(\Psi_+\)).

**Figure 4.** Out of phase overlap of two p AOs (\(\psi_a - \psi_b\)) to create a \(\sigma^*\) antibonding MO (\(\Psi_-\)).

Spartan represents phase by coloring orbitals (or lobes of orbitals) red or blue. Red represents the negative phase (or trough); blue represents the positive phase (or crest). The point or plane that an orbital changes phase (color) is called a node. If an orbital has a node no electrons are found in that area of space. (In other words, the probability of finding an electron there is zero.) Each p orbital in Figures 3 & 4 above has 1 node: a vertical plane through the center of the atom, perpendicular to the plane of the paper. The sigma (\(\sigma\)) bonding MO contains 2 nodes: each atom has a vertical plane through its center. The sigma antibonding (\(\sigma^*\)) MO contains 3 nodes: 2
vertical planes through the center of both atoms & 1 more vertical plane through the bond axis (the gray "bond").

The sigma (σ) MOs (seen in Figures 3 & 4) are created by head-to-head overlap of atomic orbitals. Another type of MOs, pi (π) MOs can be formed when p atomic orbitals undergo a side-by-side interaction (Figures 4 & 5). A node (more accurately, a nodal plane) always exists along the bond (i.e., bond axis) of a π bond. For the antibonding MO shown in Figure 6 a nodal plane also exists perpendicular to the bond axis.

![Figure 5](image1.png)

*Figure 5.* In phase overlap of two p AOs ($\psi_a + \psi_b$) to create a π bonding MO ($\Psi_+$).

![Figure 6](image2.png)

*Figure 6.* Out of phase overlap of two p AOs ($\psi_a - \psi_b$) to create a π* antibonding MO ($\Psi_-$).

The atomic orbitals and molecular orbitals in Figures 3-6 require complicated calculations and assumptions that far exceed the equation shown for $\psi_{nlm}$ on page 2. In Spartan, these orbitals are called HOMOs or LUMOs. The **HOMO (highest occupied molecular orbital)** is the valence orbital that received the last valence electron(s). The orbital directly beneath the HOMO in energy is labeled HOMO(-1). The **LUMO (lowest unoccupied molecular orbital)** is the empty orbital just above the HOMO. The orbital just above the LUMO is labeled LUMO(+1). The "1" can be changed to 2, 3, 4, ... to create a complete set of all MOs in the molecule. The HOMO and LUMO images (surfaces) created by Spartan can be correlated to or represented by the horizontal lines in the center of a molecular orbital (MO) diagram.

As stated above, molecular orbitals in a molecular orbital diagram are the horizontal lines in the center. The atomic orbitals that create these molecular orbitals are represented by the horizontal lines on each side. The **average** energy of the last filled valence atomic orbitals is assumed to be zero. Note the word “average”… For a homonuclear diatomic like N₂, the zero energy is the energy of the p atomic orbitals of the nitrogen atoms – no averaging needed because the orbitals of both nitrogen atoms are the same. However, for a heteronuclear diatomic like ´CN or CS, the
atomic orbital energies depend on atom electronegativity and/or size. (Atomic orbitals of **more electronegative atoms** are lower in energy. The larger an atom is, the closer together its atomic orbitals are (i.e. the energy difference between 2s and 2p is larger than between 3s and 3p.) As atomic orbitals move toward each other, the molecular energy grows in magnitude, becoming negative for bonding MOs: a molecular orbital that is more stable than the separate atomic orbitals forms. The stabilization results from the electrostatic attraction (→) of both electrons to both nuclei being greater than the electrostatic electron-electron or nucleus-nucleus repulsion (↔). For antibonding MOs, the opposite is true: a more unstable molecular orbital forms with a large positive energy value. **Molecular orbitals of heteronuclear diatomics typically have larger orbital lobes encompassing the atom that is closer in energy.**

![Figure 5. Electrostatic Interactions in H₂.](image)

 Furthermore, the electrons of a bonding molecular orbital occupy a larger space between the two nuclei when compared to the electrons localized around the nuclei of two separate atomic orbitals. This **delocalization** of the electrons lowers their kinetic energy (the electrons slow down), resulting in a molecular orbital that is more stable than the atomic orbitals that formed it. Conversely, electrons in antibonding orbitals move faster as they are more localized than the atomic orbitals from which they came.

Any bonding molecular orbital allows for electron delocalization compared to an atomic orbital, but a π bonding molecular orbital spread over **three or more atoms** provides even greater delocalization. This delocalization results from the existence of 2 or more resonance structures: 2 or more Lewis structures of the same molecule or ion showing different arrangements of multiple bonding (double or triple bonds) and formal charge within a molecule or ion. Molecular orbitals and bond lengths found with Spartan can be used to better understand how the actual structure of a molecule or ion relates to its resonance structures.

**In this experiment, the valence atomic orbitals for hydrogen, carbon, nitrogen, and sulfur atoms will be calculated. Molecular orbitals for H₂, N₂, CS, CN, and SCN⁻ will be investigated. The structure of SCN⁻ will be elucidated by looking at its molecular orbitals and it’s bond lengths. Turn all orbital images and MO diagrams to your TA the same week that the Sapling questions are due.**
PROCEDURES


What are the electron configurations for the following atoms: H, N, C, and S? Which electrons are the valence electrons? In this section you will create the valence atomic orbitals for H, N, C, and S and compare them.

1. Open the Spartan program.
2. On the menu bar, click File and then New Build (or ).
3. In the Model Kit in the right panel, click the Organic tab.
4. In the Model Kit, click –H to select hydrogen.
5. In the Workspace area, click anywhere to place hydrogen.
6. On the bottom right corner, select the delete tool ( ). Click on the yellow bond on the hydrogen so that it disappears. (The hydrogen atom (white ball) should be left on screen.)
7. On the menu bar, click Setup, and then Surfaces.
8. In the Surfaces window, click the Add button. Choose HOMO. Move the window out of the way, but leave it open.
9. On the menu bar, click Setup, and then Calculations.
   a. Calculate: Equilibrium Geometry with Hartree-Fock 3-21G should already be selected (both are default settings).
   b. Determine how many unpaired electrons are present on the hydrogen atom. Enter that value in the Unpaired Electrons field of the Calculations window.
   c. Click Submit to exit Calculations window and start the calculation.
10. When the Save As window appears name the file and click on Save. Click OK button to start the calculations. Almost immediately, a dialog will appear indicating that the calculations are complete. Click the OK button to clear the dialog. Leave this file open
11. Repeat steps 2-10 for the carbon atom. Remove all yellow bonds. Exception: Create the surfaces of LUMO, HOMO, HOMO -1, -2, and HOMO -3. Creating HOMO -1, -2, and -3 is accomplished by clicking on the More Surfaces button in the Surfaces window and choosing HOMO(-). Change the number in the field and click Apply for each desired orbital.
12. Repeat step 11 for the nitrogen atom.
13. Repeat steps 11 for the sulfur atom.
14. Notice the tabs at the bottom middle of the screen that correspond to each file created. Different files can be brought forward by clicking on the desired tabs. To display all 4 at the same time by clicking on the box in the tab label so that a check mark is visible. Drag each atom out of the middle of the screen (so that all the atoms do not stack up on top of each other and you can see all of them) into a neat line and order (from left to right) hydrogen (white), carbon (gray), nitrogen (purple), and then sulfur (yellow).
15. Display the s-orbitals on all 4 atoms. Change the Style of all the surfaces to Mesh by clicking on the surface and then changing the Style menu (bottom right corner of program window) from Solid to Mesh. (All surfaces in this experiment should be viewed in Mesh.) Copy the images on the screen into MS Word by going to Spartan’s Edit menu and choosing Copy. Then switch to MS Word and paste. All four images should be
pasted in one step. Label each orbital with the appropriate quantum numbers. What is responsible for the different size of these orbitals? 

16. Display one set of p-orbitals for 3 of the 4 atoms. Orient all of the orbitals in the same direction and repeat step 15.

17. Label each orbital with the appropriate quantum numbers (i.e., 2p, 3s, etc.). What is responsible for the different size of these orbitals? Close all files before continuing.

B. Finding $\Psi_{H_2}$: Diatomic Hydrogen ($H_2$) Calculations

1. Determine the Lewis structure and sketch the molecular orbital (MO) diagram of $H_2$ using the 1s atomic orbitals from the two hydrogen atoms.
2. On the menu bar, click File and then New.
3. In the Model Kit in the right panel, click the Organic tab and then click $-H$ to select hydrogen.
4. In the Workspace area, click anywhere to place hydrogen. Click on the yellow bond to add an additional hydrogen.
5. Optimize the structure. Click Build, and then Minimize.
6. On the menu bar, click Setup, and then Surfaces. Click the Add button. Choose HOMO and then LUMO. Move the window out of the way, but leave it open.
7. On the menu bar, click Setup, and then Calculations.
8. Leave the default settings: Calculate: Equilibrium Geometry with Hartree-Fock 3-21G. Click Submit to exit Calculations window and start the calculation.
9. When the Save As window appears name the file and click Save. Click OK button to start the calculations.
10. Arrange the molecule so the bond is horizontal; copy and paste the Mesh images on to MO diagram created in B.1 above. All images should be copied with the bond in the same orientation to make comparison easy and the appropriate atomic orbital(s) collected in Part A should also be included.

Only Correct Orientation: ![Correct Image]

Many Incorrect Orientations: ![Incorrect Images], et cetera.

11. Close this file before proceeding.

C. Finding $\Psi_{N_2}$: Homodinuclear Calculation ($N_2$)

1. Determine the Lewis Structure and sketch the molecular orbital diagram for $N_2$ using nitrogen atoms’ valence atomic orbitals (2s and 2p).
2. To build this molecule in Spartan, use the $\equiv N$ button in the Organic Model Kit.
   Optimize the structure, click Build, and then Minimize.
3. Perform an Equilibrium Geometry calculation with the Hartree-Fock 3-21G method to find the following molecular orbitals of $N_2$: LUMO +2 & +1, LUMO, HOMO, HOMO -1 to -4.
4. As in Part B, arrange the molecule so the bond is horizontal and copy and paste the Mesh images into the MO diagram. Label all orbitals with appropriate atomic or molecular designation (i.e., 2p_x, $\sigma_{2s}$, $\pi_{2pz}$, etc.) and the Spartan surface label (LUMO+2, HOMO -1, etc). Provide the valence molecular electron configuration and bond order.
5. Begin a table containing all of the molecular orbitals collected in part C - F. The first column on the left should contain the molecular orbital designation: $\sigma_s$, $\sigma_s^*$, $\sigma_p$, $\sigma_p^*$, $\pi$, or $\pi^*$. List these orbitals in order of descending energy. Underneath each image indicate if the orbital is LUMO +2, LUMO +1, LUMO, HOMO, et cetera. The table should be structured as follows:

<table>
<thead>
<tr>
<th>Orbital</th>
<th>N$_2$</th>
<th>SC</th>
<th>CN$^-$</th>
<th>SCN$^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_p^*$</td>
<td>![Image]</td>
<td>LUMO +2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\pi_{p^*}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\pi_{p^*}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_p$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>......</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

When copying and pasting into the table, make sure the bond axis remains horizontal and the size of the atoms stays the same.

D. Finding $\Psi_{CS}$: Heterodinuclear Calculation (CS)

1. Determine the Lewis Structure for CS. *Note:* Make sure you minimize formal charge.
2. To build this molecule in Spartan use the Inorganic Model Kit. Click on the $\rightarrow$ button and then choose C (carbon). Click anywhere in the workspace area to add the carbon. Choose S (sulfur) and add bond to the carbon in the Workspace area. Click on the $\equiv$ button. Click on the bond between the carbon and sulfur atoms until you see the triple bond. Optimize the structure, click Build, and then Minimize. Clicking on the $\equiv$ button results in a visual representation of a triple bond. However, the multiple bonds that you enter are for aesthetics. When an equilibrium geometry calculation is done, Spartan calculates bond lengths based on quantum mechanical principles. Bond lengths can then be correlated with bond order – the longest bonds are single, intermediate length bonds are double, and the shortest bonds are triple. Perform an Equilibrium Geometry calculation with the Hartree-Fock 3-21G method to find the following molecular orbitals of CS: LUMO +2 & +1, LUMO, HOMO, HOMO -1 to -4.
3. Arrange the molecule so the bond is horizontal with sulfur on the left and carbon on the right; add the orbital images to the table started in Part C, following the directions given in C.5. You do NOT need to create an MO diagram for CS, but it has the same number of valence electrons as N$_2$, so you should be able to extrapolate what it might look like from the MO diagram created in Part C.

E. Finding $\Psi_{CN}$: Heterodinuclear Calculation (CN)

1. Determine the Lewis Structure for CN.
2. To build this anion in Spartan, use the $\rightarrow$C $\equiv$ and $\equiv$N buttons in the Organic Model Kit. Delete the yellow bond on the carbon click on the delete icon ( ) and then click on the yellow bond on the carbon so that it disappears. Optimize the structure, click Build, and then Minimize.
3. Perform an **Equilibrium Geometry** calculation with the **Hartree-Fock 3-21G** method (be sure to set the **Total Charge to anion**) to find the following molecular orbitals of CN:\n\[
LUMO +2 & +1, LUMO, HOMO, HOMO -1 to -4.
\]
4. Arrange the molecule so the bond is horizontal with carbon on the left and nitrogen on the right; add the orbital images to the table started in Part C, following the directions given in C.5. You do NOT need to create an MO diagram for CN`, but it has the same number of valence electrons as N\textsubscript{2}, so you should be able to extrapolate what it might look like from the MO diagram created in Part C.

**F. Finding \( \Psi_{SCN^-} \): Heteronuclear Triatomic (SCN\textsuperscript{−}) Calculations**

**F.1 Creating the Actual Structure:**

1. Build \( \text{SCN}^- \) with the **Inorganic Model Kit**. Click on the \( \rightarrow \) button and then choose **S** (sulfur). Click anywhere in the workspace area to add the sulfur. Click on the \( \rightarrow \rightarrow \) button, choose **C** (carbon), and then add bond to the sulfur in the **Workspace** area. Click on the \( \rightarrow \) button, choose **N** (nitrogen), and then add bond to the carbon in the **Workspace** area. Optimize the structure; click **Build**, and then **Minimize**. Because two significant resonance structures exist for SCN\textsuperscript{−}, double or triple bonds will not be added here. We will let Spartan decide the real structure (which is an unequal average of the two resonance structures).

2. Perform an **Equilibrium Geometry** calculation with the **Hartree-Fock 3-21G** method to find the following molecular orbitals of SCN\textsuperscript{−} (be sure to set the **Total Charge to anion**): \( LUMO +2 \& +1, LUMO, HOMO, HOMO -1 to -7 \). Before submitting the calculation, click on the boxes to the left of **Infrared Spectra** and **Vibrational Modes** in the **Calculation** window.

3. Arrange the molecule so the bond is horizontal with sulfur on the left and nitrogen on the right; add the orbital images to the table started in Part C, following the directions given in C.5. (No MO diagram is required.) **Exceptions:**
   a. Place each SCN\textsuperscript{−} molecular orbital in the row next to the N\textsubscript{2}, CS, and CN\textsuperscript{−} orbitals showing the same type of bonding. *For example, if the SCN\textsuperscript{−} molecular orbital is a result of atomic \( p_\pi \) orbitals creating two \( \sigma \) bonds, put it in the row with the N\textsubscript{2}, CS and CN\textsuperscript{−} \( \sigma \) orbitals created from p atomic orbitals.* Place any SCN\textsuperscript{−} orbital(s) that are not similar at the bottom of the table.
   b. Label the orbitals with LUMO+2, HOMO, etc. and indicate whether the type of bonding (\( \sigma, \sigma^*, \sigma_p, \sigma^*_p, \pi, \) or \( \pi^* \) or n (nonbonding atomic orbital)) for both the S-C and the C-N bonds. *For example, indicate \( \pi, \pi \) if both bonds are \( \pi \) bonding.*
   c. Begin a table for S-C and C-N bond lengths and IR stretching frequencies.
      i. Measure the bond lengths by clicking on the gray bond until a yellow “mask” appears around the bond. The bond length will then be displayed in the bottom right corner of the program window.
      ii. Go to the **Display** menu and choose **Spectra**. Click on \( + \) and select **IR calculated**. Click on the peaks in the Spectra window. The ion will be animated to show the vibration of bond length or angle at each frequency. *Pay special attention to the frequencies that correspond to the visible peaks on the spectrum.*
Record the frequencies that result in stretching vibrations of the sulfur-carbon bond and for the carbon-nitrogen bonds.

F.2 Creating the Resonance Structures:
1. Determine the Lewis Structures of the following molecules: CH$_3$-S-CH$_3$, S=CH$_2$, H$_2$C=NH, HC≡N. Molecular geometry is important!
2. Build these molecules separately with the Inorganic Model Kit. (Calculations will incorrect if the geometry is wrong.) Choose the button corresponding to the correct geometry for each atom. Insert the double or triple bonds by choosing the bond type (= or ≡) and then double clicking on the bond. Clicking on = or ≡ buttons result in visual representations of double and triple bonds. However, the multiple bonds that you enter are for aesthetics. When an equilibrium geometry calculation is done, Spartan calculates bond lengths based on quantum mechanical principles. Bond lengths will then be correlated with bond order – the longest bonds are single, intermediate length bonds are double, and the shortest bonds are triple.
3. Optimize the structure; click Build, and then Minimize. Perform an Equilibrium Geometry calculation with the Hartree-Fock 3-21G method. Before submitting the each calculation, click on the boxes to the left of Infrared Spectra and Vibrational Modes in the Calculation window.
4. Record the C-S and C-N bond lengths and IR stretching frequencies in the table created in F.1.3c above. (Record only IR frequency for each molecule – choose the one that shows the greatest amount of C-S or C-N bond stretching.) The bond lengths will be used to create the resonance structures below.
5. Determine the two most important Lewis Structures (resonance structures) for SCN$^-$. Note: Make sure you minimize formal charge.
6. Build both resonance structures separately with the Inorganic Model Kit. Set the appropriate bond lengths for each resonance structure using the data just collected. (Choose Measure Distance from the Geometry menu. Click on the two atoms involved in the bond (or directly on the bond itself). Enter the numerical value for the bond length in the Distance field in the bottom right hand corner of the program window. Hit Enter. Do NOT optimize the structure.
7. Perform an Energy calculation with the Hartree-Fock 3-21G method for each resonance structure separately. Remember to set the Total Charge to Anion. Before submitting the calculation, click on the boxes to the left of Infrared Spectra and Vibrational Modes in the Calculation window.
8. Once the calculations are complete, check the bond lengths, they should be unchanged. (If they have changed, repeat the calculation, making sure you choose Energy instead of Equilibrium Geometry.) Go to the Display menu and choose Spectra. Click on * and select IR calculated. Click on the peaks in the Spectra window. The ion will be animated to show the vibration of bond length or angle at each frequency. Pay special attention to the frequencies that correspond to the visible peaks on the spectrum. Record the frequencies that result in stretching vibrations of the sulfur-carbon bond and for the carbon-nitrogen bonds in the table created above.
POST LAB

Log onto Sapling and complete the postlab questions. The following diagrams and tables should be turned into your TA the same week the Sapling assignment is due:

- AO Table with H, C, N, and S orbitals (Part A.)
- MO Diagrams of $H_2$ and $N_2$ with orbital images – printed in color. (Part B & C.)
- MO Table containing $N_2$, CS, CN⁻, and SCN⁻ MOs arranged by bonding type. (Part C-F.)
- Table Containing Bond Lengths and IR stretches from the equilibrium geometry calculations of SCN⁻, CH₃-S-CH₃, S=CH₂, H₂C=NH, and HCN; as well as the energy calculations of the SCN⁻ resonance structures. (Part F.)