1. Describe the difference between $\sigma$ and $\pi$ molecular orbitals. Using a diagram to explain this problem might be helpful. (5 points)

2. Describe the difference between bonding and antibonding molecular orbitals. Using a diagram to explain this problem might be helpful. (5 points)
3. Explain why the difference between the energies of the $\sigma_{2p}$ bonding and $\sigma_{2p}^*$ antibonding orbitals is larger than the difference between the $\pi_x$ or $\pi_y$ bonding and $\pi_x^*$ or $\pi_y^*$ antibonding orbitals. See the diagram below. (Hint: see section 9.8 of the text) (5 points)

4. Consider the following molecules and molecular ions: CO; CO$^+$; CO$_2^+$. For each of these molecules:
   a. The molecular orbital diagram for this molecule is slightly different in form than that shown above. For reasons discussed in your text on pages 336-337, the $\pi_x$ and $\pi_y$ orbitals are lower in energy than the $\sigma_{2p}$ orbital, as shown below.
   Write a valence molecular orbital diagram (ignoring the 1s core electron diagram), similar to the one above, for each of the 3 molecules, being sure to include the location of the electrons. (Hint: it is not necessary to write the Lewis structure for each molecule) (2 points)
   b. Calculate the bond order for the C-O bond. (2 points)
   c. Determine if the molecule or ion is paramagnetic or diamagnetic. (2 points)
   d. Place the molecule and ions in order of increasing bond length. (2 points)
   e. Place the molecule and ions in order of increasing bond strength. (2 points)

5. Show, by using a drawing, how two 2p atomic orbitals can combine to form a $\sigma$ or $\pi$ molecular bond. (5 points)

6. We have looked extensively at bonding in two types of compounds. In an ionic compound, the atoms obtain lower energy by transferring electrons and then forming a 3-dimensional crystal lattice structure. In a molecular compound, the atoms obtain lower energy by sharing electrons and forming molecules. But there are some elements or compounds that obtain lower energy states by forming an extended solid that is neither an ionic crystal nor a molecule. These types of compounds are called molecular or covalent solids. For example, elemental carbon exists as a solid in two common allotropes, diamond and graphite (and also other forms called amorphous carbon, which we will not consider here). Diamond, the hardest natural substance known, exists as neither an individual molecule nor an ionic solid. The bonding in diamond consists of tetrahedrally bonded carbon atoms each bonded to 4 other carbon atoms, arranged in a huge regular network. A unit cell of the diamond solid is shown below:
Figure 1. The diamond structure.

Each circle represents a carbon atom, and each line is a bond to another carbon atom. This unit cell, repeated in all 3 dimensions, gives the extended solid structure of diamond.

In contrast, graphite is bonded to only 3 other carbon atoms, whose bonds lie entirely within planes, making this a 2-dimensional layered solid. A section of the graphite structure is shown on the next page:

Figure 2. Two views of graphite. A: Side view of graphite showing the planar arrays of fused six-membered rings. At the corner of each ring is a carbon atom (not shown as a circle for reasons of clarity). The second layer is not aligned with the first, however. B: Top view of graphite showing how the second layer (dashed lines) is oriented with respect to the first layer (solid lines). Half of the atoms have another atom directly below them, and the other half do not.

The spacing between layers is 3.35 Å, while the distance between carbon atoms within a layer is 1.42 Å. Since the layers are held together with relatively weak forces, they can slide past one another. Graphite is a lubricant because of this property.

Buckyball (buckminsterfullerene - C_{60}) is a third allotrope of carbon. The bonding in buckyball is similar to that in graphite: each carbon atom is bonded to three other carbon atoms, and consists of 5- and 6-membered rings bonded together to form a ball of 60 carbon atoms, similar in shape to a soccer ball. A diagram of buckyball is shown at left. Notice the 5- and 6-membered rings and the single and double bonds.
Answer the following questions for each allotrope of carbon: diamond, graphite, and buckyball.

a. Consider the localized bonding model. What is the hybridization used by the carbon atoms in each allotrope of carbon. (2 points)
b. Determine the bond order for a C-C bond in each allotrope of carbon. (3 points)
c. Which of the structures (if any) would require resonance structures. Explain. (2 points)
d. The bond energy for a C-C single bond and a C=C double bond are shown on the next page. The bond energy is the energy released when separated carbon atoms in the gas phase come together to form 1 mole of C-C bonds.

<table>
<thead>
<tr>
<th>Bond</th>
<th>Bond Energy (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-C</td>
<td>-347</td>
</tr>
<tr>
<td>C=C</td>
<td>-614</td>
</tr>
</tbody>
</table>

Calculate the expected amount of energy released when 1 mole of carbon-carbon bonds are formed for each of the allotropes of carbon. (Hint: on average, how many C-C single bonds and C=C double bonds will there be in 1 mole of graphite or buckyball bonds.) (3 points)
e. Based on your answer to Problem d., what do you predict to be the least stable (highest energy) form of carbon? Does this surprise you? (1 point)
f. In fact, the energy released upon the formation of 1 mole of graphite and 1 mole of buckyball bonds is NOT the same (don't change your answer to Problem d.). One way to compare the energy of the bonds in graphite and buckyball is to burn 1 mole of each compound in oxygen to form CO₂, and measure the energy released (calorimetry). When 1 mole of carbon in graphite form is burned in O₂, -394 kJ/mol of energy is released. When 1 mole of graphite in buckyball form is burned in O₂, -435 kJ/mol of energy is released. Although it might seem that buckyball is actually lower in energy than graphite, if you examine a modified Born-Haber diagram (an energy diagram) for the burning process, you can see that C₆₀ is actually higher in energy (a less stable form of carbon):

To figure out why there is a difference when the bonding seems the same, answer the following questions: (1 point each)
1. According to the VSEPR theory, what is the predicted bond angle around any carbon in either graphite or buckyball. A piece of each allotrope is shown at right.
2. Draw resonance structures for the piece of buckyball/graphite shown at right.
3. How many $\sigma$ and how may $\pi$ bonds will there be around any carbon atom in buckyball and graphite.

4. Consider the delocalized (molecular orbital) bonding model. Describe what the $\pi$ molecular orbitals might look like in buckyball/graphite. A picture might be helpful. (Hint: in Problem 2, was the double bond you drew localized between any 2 particular carbon atoms?)

5. Consider the 3-D structure of buckyball and graphite. The bonds in one of these structures will NOT be as you predicted in Problem 1. Which one is it and why? (Hint: you might think of buckyball as being formed by taking a planar sheet of graphite and shaping into a sphere)

6. Considering bond energy and the information in Problem f., which C-C bond (in buckyball or graphite) do you think is stronger (lower energy)?

1. Put it all together: Rationalize why buckyball bonds are weaker than graphite bonds. Here are some hints: A weaker bond is closer to being broken (takes less energy to break) than a stronger bond. The bonds in buckyball and graphite are both C-C with the same hybridization and $\sigma$ and $\pi$ bonding, but the buckyball bonds are closer to being broken than they are in graphite. What if someone gave you two sticks and asked you to break them by bending them in half. One stick is straight, and the other is a stick that has been partially bent for you. Which one will break with less effort (energy)?

We said that nature always wants to be in its lowest energy state. If this makes you wonder why diamonds don't just transform into more stable graphite, take more chem!