Question 1 For the molecular formula C₃H₄Br₂:

a) Give the degrees of unsaturation.

b) Draw TWO PAIRS of stereoisomers. Your structures can be Lewis or line-angle, your choice. INCLUDE ALL NON-BONDING ELECTRONS.

c) Draw FOUR more structural isomers. NONE OF THESE FOUR STRUCTURAL ISOMERS CAN BE THE SAME AS ANY OF THOSE STRUCTURES YOU DREW IN ANSWER TO QUESTION b) ABOVE. Your structures can be Lewis or line-angle, your choice. INCLUDE ALL NON-BONDING ELECTRONS.

Question 2 For the following three anions:

a) Give the hybridization of the atomic orbital containing the non-bonding electrons and draw a picture of its wavefunction on top of each anion.

```
H\(-\text{C:O}\)  \(\text{H}\) \(\text{H}\)  \(\text{H}\)
A

\(\text{H}\) \(\text{C}\=\text{C:O}\)  \(\text{H}\)  \(\text{H}\)
B

\(\text{H}\) \(\text{C}\equiv\text{C:O}\)  \(\text{H}\)  \(\text{H}\)
C
```

b) Rank the ions in order of INCREASING ionization potential. Give a BRIEF explanation

\text{lowest} \quad \text{_____} \quad < \quad \text{_____} \quad < \quad \text{_____} \quad \text{highest}
Question 3: For each structure pair A and B:

a) Draw the MOLECULAR dipole moment ON TOP OF THE STRUCTURES. Your drawings of the dipole moments do not need to indicate the sizes of the moments (give that information in your explanation, below), just the approximate directions.

b) For A and B, clearly state which is the largest BOND DIPOLE moment in each structure

c) BRIEFLY explain which has the larger molecular dipole moment and why. Your explanations should include discussion of at least some of the factors that determine the magnitudes of the bond dipole moments, as appropriate

\[
\begin{align*}
A & : \text{H}_3\text{C} - \text{C} = \text{N} : \\
B & : \text{H}_3\text{C} - \text{CH} = \text{N} : 
\end{align*}
\]

A has the larger molecular dipole moment because the C-N triple bond dipole moment is larger than the C-N double bond dipole moment because of the larger degree of polarization of the electrons in the triple bond (more \(\pi\)-electrons), and also because of the bond dipole moment in the N-H bond in B partially opposes the C=N dipole moment.

There is only 1 substantial bond dipole moment in A, which is that for the C-N triple bond

There are 2 substantial bond dipole moments in B, that for the C=N double bond is larger than that for the H-N single bond because electrons in \(\pi\)-orbitals are more polarizable than electrons in \(\sigma\)-orbitals because they are further away from the nuclei and are held less "tightly"

Question 4: In the following line-angle structures, circle and identify all functional groups, ignore alkanes (alkyl groups) (non-bonding electrons omitted for clarity)

adrenaline

Question 5: Give one property of electrons that can only be explained by taking into account their wave behavior

• we can only explain the formation of both bonding and anti-bonding molecular orbitals this way

• the wave behavior requires quantization of electron energies, which forces them to occupy distinct orbitals, this is why we have orbitals, if we have no wave behavior, we have no orbitals!

• the fact that we can only give a probability of finding an electron in a particular position is a consequence of the wave behavior

Extra Credit: In the "Organic Chemistry in Real Life" pages, which of the following biological molecules was discussed in terms of energy storage?

NADH DNA ATP AMP
Question 6:
a) Determine the degrees of unsaturation for the condensed structure CH₂CN. Draw a Lewis structure for this molecule, show all lone pairs (non-bonding electrons). Indicate the hybridization at both carbons and the nitrogen atom for the structure that you drew.

b) Draw a 3-D structure of the molecule that illustrates clearly all of the bond angles in this molecule and give ALL of the bond angles. Use dashed/wedged formalism as appropriate.

c) Redraw your molecule and show clearly the $\Psi$ of the localized C-N $\sigma$-bonding molecular orbital. Indicate the A.O.'s used to construct the molecular orbital.

e) Do the same for one of the carbon nitrogen $\pi$-bonding molecular orbitals.

e) Do the same for one of the localized carbon hydrogen $\sigma$-bonding molecular orbitals.
Question 7: Rank the three bonds A, B and C as indicated with the arrows in order of INCREASING bond dissociation energy (not all H atoms included in the line-angle structure) and give a brief explanation that includes the term "energy of the electron(s)"

A \quad B \quad C

\begin{align*}
\text{smallest BDE} & \quad < \quad \text{___} & \quad < \quad \text{___} & \quad \text{largest BDE}
\end{align*}

carbon-hydrogen bonds are stronger than carbon-carbon bonds because they are built using the smaller 1S A.O. on hydrogen, that results in better atomic orbital overlap, and lower energy electrons in the bonds, so bond B has the smallest BDE.

bond A is built using a carbon sp3 A.O. compared to a carbon sp A.O. in C, the sp A.O. is smaller and lower in energy than the sp3 A.O., the electrons in bond C are lower in energy, it costs more energy to break bond C, C has the largest BDE.

---

Question 8: Convert the following condensed structure into a line-angle structure (include all non-bonding electrons)

\[
\text{CH}_3\text{CH}_2\text{CH(CH}_3\text{)(CH}_2\text{)}_2\text{CH(NH}_2\text{)CH}_2\text{OH}
\]

---

Question 9: Lavender oil is mainly linalyl acetate, with molecular formula C\text{\textsubscript{12}}H\text{\textsubscript{20}}O\text{\textsubscript{2}}. Circle the structure of linalyl acetate (*hint: think degrees of unsaturation*)

\[
\begin{align*}
\text{Structure 1} & \quad \text{Structure 2} & \quad \text{Structure 3}
\end{align*}
\]
Question 1: Identify each of the following pairs of structures as the same, stereoisomers or structural isomers

![Chemical structures](attachment:image.png)

Question 2: Each of the following structures are missing pairs of non-bonding electrons, all formal charges are provided. Add the missing non-bonding electrons, give the hybridization of the atomic orbitals that contain them, and for each structure indicate which of the pairs is highest in energy and give a BRIEF explanation for your choice of highest energy pair.

![Chemical structures](attachment:image.png)

Question 3: What does the shading mean when we draw pictures of the wavefunction of the orbital?
Question 4: For the molecular formula C₅H₁₀
a) Give the degrees of unsaturation

b) draw ONE PAIR of stereoisomers, indicate which is the cis- and which the trans-isomer

c) draw six additional structural isomers (none of which can be part your answer to part b)

Question 5: Which has the highest energy electrons, the amide anion or the hydroxide anion, give a BRIEF explanation.

\[ \text{amide} \quad \text{hydroxide} \]

Question 6: In the following line-angle structure, circle and identify all functional groups, ignore alkanes (alkyl groups). Non-bonding electrons are not shown for clarity.
Question 7: Given the drawing of the 3s atomic orbital provided
a) give a plot of the magnitude of the wavefunction ($\Psi$) versus distance from the nucleus ($r$), in two (opposite) directions as indicated by the provided axes
b) give a plot of the magnitude of the wavefunction SQUARED ($\Psi^2$) versus distance from the nucleus ($r$), in two (opposite) directions as indicated by the provided axes
c) state the number of nodes and clearly indicate the positions of the nodes on your wavefunction plot
d) clearly indicate the positions in space where the probability of finding the electrons are zero in your probability plot.
Question 7: For the two structures provided, explain which would have the larger molecular dipole moment (you do not need to draw the dipole moments).

A

\[ \begin{array}{c}
\text{Cl} \\
\text{C} \\
\text{Cl}
\end{array} \]
\[ \begin{array}{c}
\text{C} \\
\text{C} \\
\text{H}
\end{array} \]

B

\[ \begin{array}{c}
\text{Cl} \\
\text{C} \\
\text{Cl}
\end{array} \]
\[ \begin{array}{c}
\text{H} \\
\text{H}
\end{array} \]

Extra Credit: In the "Organic Chemistry in Real Life" pages, which of the following was described as the main ingredient of natural gas?

- benzene
- acetylene
- ethane
- methane
Question 1: Convert the following line-angle structure into a condensed formula

\[ \text{CH}_{2}\text{CH(CH}_{3}\text{)CH}_{2}\text{CH}_{2}\text{CO}_{2}\text{CH}_{2}\text{CH}_{2}\text{CH(CH}_{2}\text{CH}_{3}\text{)}\text{CH(OH)}\text{CH}_{2}\text{CH}_{3} \]

Question 2: For the molecular formula C\textsubscript{4}H\textsubscript{8}O:

a) Give the degrees of unsaturation.

b) Draw TWO PAIRS of stereoisomers. Your structure should INCLUDE ALL NON-BONDING ELECTRONS.

Question 3: For the structure provided, label the functional groups and give the hybridizations of the following specific atoms:

a) the carbon attached to the alcohol functional group
b) both oxygen atoms in the ester (ignore minor resonance contributors).
c) the nitrogen in the amine
d) the nitrogen in the nitrile (ignore minor resonance contributors).
Question 4: For the molecular formula $C_4H_8$

a) Give the degrees of unsaturation

b) draw ONE PAIR of stereoisomers, indicate which is the cis- and which the trans-isomer

c) draw three additional structural isomers (none of which can be part your answer to part b)

Question 5: What information do we get by taking the wavefunction squared, and why is the wavefunction squared not shaded?

Extra Credit: In ONE SENTENCE, state at least one thing that is wrong with this picture. (From O-Chem in Real Life page on Quantum Mechanics).
Question 6: In the following line-angle structure, circle and identify all functional groups, ignore alkanes (non-bonding electrons not included for clarity).

[Structural diagram]

Question 7: Rank the three indicated bonds to the hydrogens Ha, Hb, Hc (not all H atoms shown in this line-angle structure), in order of increasing bond dissociation energy and give a brief explanation that should include the term "energy of the electron(s)."

[Diagram with Ha, Hb, Hc labeled]

\[
\text{smallest BDE} \quad < \quad < \quad \text{largest BDE}
\]

Question 8: Rank the indicated pairs of electrons in order of increasing energy, give a brief explanation for your choice.

[Diagram with A, B, C labeled]

\[
\text{lowest} \quad < \quad < \quad \text{highest}
\]
Question 8: For each structure pair A and B:

a) Draw the MOLECULAR dipole moment ON TOP OF THE STRUCTURES. Your drawings of the dipole moments do not need to indicate the sizes of the moments (give that information in your explanation, below), just the approximate directions.

b) For A and B, clearly state which is the largest BOND DIPOLE moment in each structure.

c) BRIEFLY explain which has the larger molecular dipole moment and why. Your explanations should include discussion of at least some of the factors that determine the magnitudes of the bond dipole moments, as appropriate.
Question 1: For the molecular formula C₂H₅NO:

a) Give the degrees of unsaturation.

b) In EACH of the boxes A and B, draw a pair of STEREOISOMERS with molecular formula C₂H₅NO. The two pairs of stereoisomers must be different. Your structures can be Lewis or line-angle, your choice. **INCLUDE ALL NON-BONDING ELECTRONS.**

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>stereoisomer PAIR #1</td>
<td>stereoisomer PAIR #2</td>
</tr>
</tbody>
</table>

c) In box C, draw FIVE more structural isomers of C₂H₅NO. Do not use any structure that appeared in Boxes A or B in Box C. Your structures can be Lewis or line-angle, your choice. **INCLUDE ALL NON-BONDING ELECTRONS.**

<table>
<thead>
<tr>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 structural isomers (no structures here can also appear in either box A or box B)</td>
</tr>
</tbody>
</table>
Question 3: On each structure A, B and C:

a) Draw the MOLECULAR dipole moment ON TOP OF THE STRUCTURES. Your drawings of the dipole moments do not need to indicate the sizes of the moments (give that information in your explanation, below), just the approximate directions.

b) Clearly state which is the largest BOND DIPOLE moment in each structure

c) RANK A, B and C in order of INCREASING molecular dipole moment. Give a BRIEF explanation for your ranking AND for the direction of the molecular dipoles you drew, the discussion should mention the bond dipole moments as appropriate

In A, the C-Cl bond dipole is smaller than the C-F dipole (electronegativity difference), the molecular dipole is smallest of all since the C-Cl dipole exactly opposes the C-F dipole.

In B, the C-F and C-Cl dipoles add in the direction upper left to lower right. The C-F dipole is larger, hence the molecular dipole points more along the C-F bond direction.

In C, the C-F and C-Cl dipoles add in the direction left to right, more so than in B because their direction is closer (vector addition). The C-F dipole is larger, hence the molecular dipole points more along the C-F bond direction.

In A, the C-Cl bond dipole is smaller than the C-F dipole (electronegativity difference), the molecular dipole is smallest of all since the C-Cl dipole exactly opposes the C-F dipole.

In B, the C-F and C-Cl dipoles add in the direction upper left to lower right. The C-F dipole is larger, hence the molecular dipole points more along the C-F bond direction.

In C, the C-F and C-Cl dipoles add in the direction left to right, more so than in B because their direction is closer (vector addition). The C-F dipole is larger, hence the molecular dipole points more along the C-F bond direction.

The largest bond dipole moment in each structure is that associated with the C-F bond.

Question 2: For homolytic cleavage of the C-Ha and the C-Hb bonds in the structure shown, draw energy diagram as a function of C-H bond separation distance, both using the same axes provided, indicate which diagram refers to which bond cleavage. Indicate the bond dissociation energies (BDE) on your diagrams. Briefly explain which BDE would be larger and why.

Energy

C-H separation distance

Homolytic bond dissociation forms a tertiary radical for C-Ha and a secondary radical for C-Hb, the non-bonding electron in a tertiary radical is lower in energy than on a secondary radical.
Question 4:

a) For the nitrogen atom indicated in the molecule below, complete the table summarizing the hybridized (or unhybridized) atomic orbitals that the nitrogen uses to accommodate the electrons that it owns and/or shares, and exactly how the nitrogen uses the orbitals.

<table>
<thead>
<tr>
<th>orbital</th>
<th>how orbital is used</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

b) For EACH of the orbitals in the table, draw a picture of the $\Psi$ that corresponds to how the orbital is used. Redraw the molecule as many times as necessary in a way that allows you to properly draw each $\Psi$ on top of the structure. Indicate which drawing refers to which orbital. When describing bond formation, be sure and indicate exactly which atomic orbitals are used from both atoms as appropriate.
Question 6: For the Lewis structure of Vitamin C, provide the following:
   a) the missing non-bonding electron pairs (there are no formal charges in this structure)
   b) the hybridization of the atoms indicated by the arrowsetc)
   c) the approximate values of the angles that are indicated by the $\alpha$ symbol.

![Lewis structure of Vitamin C]

Question 7: Why are electrons in covalent bonds lower in energy than those not in bonds?

Question 8: Convert the following into condensed formulae and give the degrees of unsaturation.

a) \((\text{CH}_3)\text{CHCH(CH}_2\text{OH})\text{CH}_2\text{COCH}_2\text{CH}_3\)
   2 degrees (elements) of unsaturation (2 double bonds)

b) \((\text{CH}_3\text{CH}_2\text{CH(CH}_3)(\text{CH}_2\text{)}\text{CH(CH}_2\text{CH}_2\text{NH}_2)\text{CHCHCCCH}_3\)
   3 degrees (elements) of unsaturation (1 double bond and 1 triple bond)

Extra Credit: In the "Organic Chemistry in Real Life" pages, which of the following biological molecules was discussed in terms of energy storage?

NADH    DNA    ATP    AMP
Question 1: Rank the three indicated C-C bonds, A, B, C, in order of INCREASING bond dissociation energy. Give a BRIEF explanation.

Question 2: Assign the following pairs of structures as the same, stereoisomers or structural isomers.

Extra Credit: In ONE SENTENCE, state at least one thing that is wrong with this picture. (From O-Chem in Real Life page on Quantum Mechanics).
Question 1: Circle and identify all of the functional groups in Allegra (non-bonding electrons not included for clarity)

![Fexofenadine - Allegra](image)

Question 2: For the molecular formula C₂H₄O, indicate the degrees of unsaturation and provide **THREE** structural isomers. Include all non-bonding electrons.

- \( \text{C}_2\text{H}_4\text{O} \)

Question 3: Add all missing formal charges to the structures shown (all non-bonding electrons are included)

a) \( \text{H}_3\text{C} \overset{.}{\text{N}}=\overset{.}{\text{N}}=\overset{.}{\text{N}}^+ \)

b) \( \text{H}_2\text{C}=\overset{.}{\text{N}}=\overset{.}{\text{C}}=\text{CH}_3 \)

c) \( \text{O} \overset{.}{\text{O}} \overset{.}{\text{O}} \)
Question 6: Identify and draw the Ψ® for the p M.O. and the non-bonding electrons these two structural isomers of C₂H₅N

![Lewis structures](image1)

Question 7: Draw the Lewis structure for the cyclic ether that has the molecular formula C₃H₄O that contains ONE C=C double bond ONLY. For the structure that you drew, identify the HIGHEST energy electrons, and the LOWEST energy electrons. IGNORE the electrons in any sigma bonds to hydrogen atoms. Indicate the nature of the orbitals that contain the electrons.

![Lewis structures](image2)
Question 8:
a) For the two bonds indicated, give the PRODUCTS of homolytic bond dissociation and show the curved arrow pushing that describes bond dissociation

[Diagram of homolytic bond dissociation]

b) Give a SINGLE energy diagram showing homolytic dissociation of these two bonds on the same diagram, indicate which diagram refers to which bond cleavage, indicate the bond dissociation energies on the diagram and briefly explain which would be larger

[Energy diagram with separation distance on the x-axis and energy on the y-axis]

Extra Credit: In the "Organic Chemistry in Real Life" pages, which of the following was described as the main ingredient of natural gas?

benzene  acetylene  ethane  methane