Person on your **LEFT** (or **Aisle**)

- PRINT YOUR NAME ON EACH PAGE!
- READ THE DIRECTIONS CAREFULLY!
- USE BLANK PAGES AS SCRATCH PAPER
- work on blank pages will not be graded...
- WRITE CLEARLY!
- MOLECULAR MODELS ARE ALLOWED
- DO NOT USE RED INK
- DON'T CHEAT, USE COMMON SENSE!

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<table>
<thead>
<tr>
<th>H</th>
<th>Li Be</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na Mg</td>
<td>Al Si P S Cl Ar</td>
</tr>
<tr>
<td>K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr</td>
<td></td>
</tr>
<tr>
<td>Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe</td>
<td></td>
</tr>
<tr>
<td>Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn</td>
<td></td>
</tr>
</tbody>
</table>

**Interaction Energies, kcal/mol**

<table>
<thead>
<tr>
<th>H/H</th>
<th>~1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>H/Me</td>
<td>~1.4</td>
</tr>
<tr>
<td>Me/Me</td>
<td>~2.6</td>
</tr>
<tr>
<td>Me/Me</td>
<td>~0.9</td>
</tr>
<tr>
<td>Et/Me</td>
<td>~0.95</td>
</tr>
<tr>
<td>i-Pr/Me</td>
<td>~1.1</td>
</tr>
<tr>
<td>t-Bu/Me</td>
<td>~2.7</td>
</tr>
</tbody>
</table>

**Infrared Correlation Chart**

- **O-H**
  - 3300
  - 3000–3100
  - 2720–2820
  - 2 peaks

- **N-H**
  - 3300
  - broad with spikes ~3300
  - broad ~3300

- **C≡O**
  - 1720–1735
  - 1650

- **C=O**
  - 2200

- **C=CH**
  - 2200

- **C≡CH**
  - 1710
  - 1650

- **C=NR**
  - 1500

**Approximate Coupling Constants, J (Hz), for \(^1H\) NMR Spectra**

- **H-H**
  - ~7

- **H-C**
  - ~8

- **C-C**
  - ~2

- **C-H**
  - 2200

**NMR Correlation Charts**

- **Amine** \(-\text{NH}2\)
  - variable and condition dependent, ca. 2 - 6 δ

- **Alcohol** \(-\text{OH}\)
  - dependent, ca. 2 - 6 δ

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**Extra Credit** /5

**Total (incl Extra)** /175+5
Question 1 (14 pts.)
a) Give a line-angle structure for the following condensed formula. Do not forget to add all non-bonding electrons where appropriate.

\[(CH_3CH_2)_2CH(CH_2)_2COCH_2CCCHO\]

Question 2 (30 pts.) Directly ON TOP of the structures below
a) Draw a picture of the \( \Psi \) or \( \Psi^2 \) as requested, for the indicated orbitals
b) Clearly indicate the atomic orbital or orbitals that you used to construct the requested orbitals
c) For each drawing, clearly indicate the positions of any nodes, or locations of zero probability of finding the electrons, as appropriate to the question

\[\Psi^2 \text{ for the C-O } \pi^* \text{ M.O.}\]

\[\Psi \text{ for the C-Cl } \sigma^* \text{ M.O.}\]

\[\Psi \text{ for the C-C } \sigma \text{ M.O.}\]

Extra Credit (5 pts). One of the factors that contributes to the "stiffness" of the poly-peptide chains in proteins is........
Question 3 (24pts.) For the structure shown on the right:

a) give the hybridization for the nitrogen atom

b) list all of the valence atomic orbitals formally associated with this nitrogen atom and give a brief description of how the nitrogen atom uses each orbital, e.g. p atomic orbital used to make a sigma bond to chlorine (this is obviously not correct, it is just to indicate how to answer this question)

c) Give the approximate C-N-H bond angle indicated in the structure above with the arrow, assign the geometry around the nitrogen atom, AND, give a BRIEF explanation (2-3 sentences MAX.) for your choice of geometry that includes the terms "energy of the electrons", "VSEPR", "electron domains".

Question 4 (15 pts.) Circle and identify all functional groups in the following structures, ignore alkyl groups.

ibuprofen
the active ingredient in Motrin

acetaminophen
the active ingredient in Tylenol
Question 5) (48 pts.) For the molecular formula $\text{C}_3\text{H}_6\text{O}_2$

a) Give the degrees of unsaturation

b) Draw **EIGHT** structural isomers for $\text{C}_3\text{H}_6\text{O}_2$ that obey the normal rules of valence for each atom. Include all non-bonding electrons. You can draw Lewis structures or line-angle structures (your choice). If you draw line-angle structures, don't forget to include the H atoms that are normally included as part of the functional groups.

c) Draw **TWO PAIRS** of stereoisomers for $\text{C}_3\text{H}_6\text{O}_2$ that obey the normal rules of valence for each atom. Include all non-bonding electrons. You can draw Lewis structures or line-angle structures (your choice). If you draw line-angle structures, don't forget to include the H atoms that are normally included as part of the functional groups.

**DO NOT INCLUDE ANY STRUCTURES in part c) THAT WERE DRAWN AS PART OF YOUR ANSWER TO PART b) OF THIS QUESTION!!**
Question 6) (30 pts) For the structure provided:

a) Draw ALL reasonable missing resonance contributors
b) Draw the curved arrow-pushing that indicates how the electrons are delocalized
c) give the NUMBER OF ELECTRONS that are delocalized
d) Indicate which is the MAJOR resonance contributor and give a BRIEF EXPLANATION for your choice. If there are equal major contributors, indicate so.
e) Include resonance arrows and brackets to complete your description of the final structure
f) Based on the resonance contributors you drew, give the "actual" resonance hybrid structure. Indicate the atoms that have a partial charge, do not worry about determining absolute partial charges, just use the $\delta$ charge notation.

\[
\begin{align*}
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
\end{align*}
\]

\[
\begin{align*}
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
\end{align*}
\]

g) On the structure below (same one as above), give the hybridization of EVERY CARBON ATOM and also the NITROGEN ATOM. Take ALL of the resonance contributors your drew above into account when determining hybridizations.

\[
\begin{align*}
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
\end{align*}
\]

Question 7) (14 pts) One of the two carbon atoms in the C=C double bond in the structure below has a small partial negative charge. Draw a MINOR resonance contributor that illustrates which carbon this is, and clearly indicate the carbon that has this small partial negative charge. Include curved arrow pushing, resonance arrows and resonance brackets.

\[
\begin{align*}
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
&\text{C} \\
&\text{N} \\
\end{align*}
\]