Fall Workshop #4

Question #1
Name or draw each of the following structures (you may need to use your text for some of these):

3-isobutyl-4-bromooctanal
1,1-dichloro-4,4-dimethoxy-2-heptanone
1,5-dichloro-1,4-dimethoxy-2-heptanone
(E)-3-bromo-4-isopropyl-3-heptenoic acid
ethyl 3,3-dichloro-2-methoxyhexanoate
5-tert-butyl-1-allyl-1-cyclohexene
3-cyclobutyl-2-cyclopentenone
N-ethyl-3-aminocyclopentanecarboxaldehyde
N,N-diethyl-3-aminocyclopentanecarboxylic acid
2,2-diethyl-3-oxo-pentanal
4-hydroxy-5-iodo-3-azaecyclopentanone
3-chloro-3-methyl-2,4-heptanedione
(E)-5-tert-butoxy-4-isopropyl-2-decenoyl bromide
Question #2
In round-robin fashion and using the molecule shown below,

a. Identify as many functional groups as you can (use the inside cover of your text as a guide)

b. Draw dipole arrows to show all polar covalent bonds.

c. Find all of the possible H-bond accepting groups.

d. Find all of the possible H-bond donating groups.

![Molecule Diagram]

Question #3
Discuss as a group the 4 major types of intermolecular interactions (VDW forces, dipole-dipole, hydrogen-bonding, and ion-dipole) that exist in the first system described below (flask of pure ethanol). Then, each student should select one of the subsequent systems (b-g) and describe the type(s) of IM forces that will exist in each of the following examples. Be sure to draw a picture to illustrate EACH of the possible intermolecular interactions.

(a) a flask of pure ethanol

(b) a flask of pure dichloromethane (a.k.a. methylene chloride)

(c) a flask of pure carbon tetrachloride

(d) a flask of pure cyclohexane

(e) a flask of pure acetone

(f) an aqueous solution of ethanol

(g) an aqueous solution of ethanoic acid

(h) an aqueous solution of NaCl

(i) a mixture of diethyl ether and ethanol
Question #4
Take a few minutes and compose an answer to each question including a brief explanation of the principle that frames your response. After the allotted time, discuss your answer as a group.

a. Why is dimethyl ether COMPLETELY soluble in water, but diethyl ether is only SLIGHTLY soluble in water, and di-tert-butyl ether is essentially INSOLUBLE in water?
b. Why is methanol (MW = 32 g/mol) a liquid at room temperature, while propane (MW = 44 g/mol) is a gas?
c. Why does 2-hexanone (bp = 127 °C) have a higher boiling point than 2,2-dimethyl-1-aminopropane (bp = 85.5 °C)?
d. Why is 1-decanol completely insoluble in water whereas ethanol is highly soluble in water?
e. Rank the following compounds in order of INCREASING boiling point.

![Chemical Structures]

f. Rank the compounds shown above in order of DECREASING solubility in water.
g. Which compound is more soluble in water: acetic acid or acetaldehyde? Explain.

Question #5
Given the Newman projection shown below (eclipsed conformation) and the table of strain energy, answer the following questions. You will want to build this compound using your model kit.

<table>
<thead>
<tr>
<th>Type of Interaction</th>
<th>Strain Energy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H, H eclipsing</td>
<td>0.9</td>
</tr>
<tr>
<td>H, CH₃ eclipsing</td>
<td>1.2</td>
</tr>
<tr>
<td>H, CH₂CH₃ eclipsing</td>
<td>1.5</td>
</tr>
<tr>
<td>H, CH(CH₃)₂ eclipsing</td>
<td>1.9</td>
</tr>
<tr>
<td>CH₃, CH₂CH₃ eclipsing</td>
<td>2.6</td>
</tr>
<tr>
<td>CH₃, CH₂CH₃ gauche</td>
<td>1.2</td>
</tr>
<tr>
<td>CH₃,CH(CH₃)₂ eclipsing</td>
<td>3.4</td>
</tr>
<tr>
<td>CH₃, CH(CH₃)₂ gauche</td>
<td>1.8</td>
</tr>
</tbody>
</table>

(a) Calculate the potential energy for the given Newman projection.
(b) Which of the following best describes the interaction indicated by the BOX in the Newman projection above (circle your choice)?

1. torsional strain
2. steric strain
3. angle strain
4. both torsional and steric strain
5. both steric and angle strain
6. both torsional and angle strain

(c) Draw the Newman projection that would result from the 60° rotation of the BACK portion of the molecule (indicated by the arrow above) about the central C-C bond of the original Newman projection.

(d) Calculate the potential energy for this Newman projection.

(e) Which of the two conformations will most likely predominate at equilibrium? You can calculate an equilibrium constant using \( \Delta E = -RT \ln K_{eq} \) Assume here that the sample exists at room temperature (27 °C) and that \( R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1} \). Show your work and explain how the values for \( \Delta E \) and \( K_{eq} \) agree.

\[ \text{E} \quad \text{S} \]

\( \text{E} = \text{eclipsed}, \text{S} = \text{staggered} \)