1. energies / 18
2. f groups / 18
3. dipoles / 22
4. bde / 22
5. isomers / 20
6. M.O. / 20
7. hybrid / 22

Interaction Energies, kcal/mol

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

Infrared Correlation Chart

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

NMR Correlation Charts
Question 1 (20 pts) Rank the indicated pairs of electrons A, B, C and D in order of INCREASING energy. Give a BRIEF explanation. (the points are for the explanation, not for getting the order correct)

A non-bonding
B non-bonding
C σ-bonding
D σ-bonding

non-bonding electrons are higher energy than bonding electrons, so A + B > C + D, A are in sp3 hybridized A.O., B in an sp hybrid A.O., sp3 more p character thus A are highest energy. The electrons in C are in a M.O. that was "built" from an sp3 and an sp hybrid A.O., compared to D which is sp3 + sp3, thus C are lowest of all

grading, mostly common sense, 1/2 correct for 1/2 points etc, 4 pts for correct order

Question 2 (14 pts) Circle and identify all of the functional groups in the provided structure. The structure is shown in its neutral form, there are no formal charges. (ignore alkyl chains, and you do not have to specify primary, secondary or tertiary if relevant)

thyroxine
a thyroid hormone that regulates metabolism

carboxylic acid
ether
aromatic
amine
alcohol

halide can be used in place of iodide

Extra Credit (5 pts.) BRIEFLY give ONE way in which anti-bonding orbitals are used by organic molecules

they accept electrons in chemical reactions AND they are where the electrons "go to" upon photochemical excitation
Question 3 (22 pts) For the structures A, B and C, indicate the molecular dipole moments ON TOP OF EACH STRUCTURE and RANK them from smallest to largest (do not try to indicate their relative size using arrow length). Give a BRIEF explanation. YOUR EXPLANATION SHOULD INCLUDE THE TERM "BOND DIPOLE MOMENT(S)"

![Chemical Structures](image)

- **A**: Oxygen is more electronegative than S, will polarize the electrons in the π-bond more, bonds to O will have larger BOND dipole moments.
- **B**: In A the 2 C=O bond dipoles add to give the largest molecular dipole moment, in C the 2 C=S bond dipoles add to make the smallest molecular dipole and B is in the middle.

Question 4 (24 pts.) For the structure below
a) Add the curved arrow-pushing that describes homolytically cleavage of the O-Ha bond (ONLY), and draw the products of bond cleavage (include all non-bonding electrons).

![Chemical Reaction](image)

b) BRIEFLY explain which of the two bonds O-Ha and C-Hb would have the largest bond dissociation energy, include the term "energy of the electron(s)" in your explanation.

In the O-H bond the electrons are lowest in energy since both "see" the most electronegative element oxygen. Breaking the O-H bond raises the energy of the electrons in the bond the most, the BDE fo O-Ha is larger than that for C-Hb.

c) Using the axes provided, draw an ENERGY DIAGRAM for cleavage of the O-Ha and C-Hb bonds ON THE SAME DIAGRAM (you can normalize your diagrams where you like).

d) Indicate the MAGNITUDES of the two bond dissociation energies on your diagrams.
Question 5 (40 pts) For the molecular formula $C_4H_8O$:

a) Give the degrees of unsaturation.

```
max # of hyrdogens = (4 x 2) + 2 = 10
actual # of hydrogens = 8
degrees = (10 - 8) / 2 = 1 degree
```

b) In EACH of boxes A and B, draw a pair of STEREOISOMERS with molecular formula $C_4H_8O$ that obey the normal rules of valence. The two pairs of stereoisomers must be different. Your structures can be Lewis or line-angle, your choice. INCLUDE ALL NON-BONDING ELECTRONS.

```
A
stereoisomer PAIR #1

B
stereoisomer PAIR #2

and many others...

and many others...
```

c) In box C, draw FIVE more structural isomers of $C_4H_8O$ that obey the normal rules of valence. Do not use any structure that appeared in Boxes A or B. Your structures can be Lewis or line-angle, your choice. INCLUDE ALL NON-BONDING ELECTRONS.

```
C
5 structural isomers (no structures here can also appear in either box A or box B)

and many others...
```
Question 6 (30 pts.) Directly ON TOP of the structures shown, draw a picture of the \( \psi \) or \( \psi^2 \) as requested, for the indicated orbitals. All non-bonding electrons and formal charges are shown. 
also give the atomic orbitals that are used to "build" the molecular orbitals as appropriate 
in each case indicate the positions of all NODES, or positions where the probability of 
finding the electrons is zero, as appropriate

\[ \text{a)} \]

\[ \text{b)} \]

Question 7 (25 pts.) For the provided structure:

a) assign the hybridization for the circled carbon atom below
b) draw a picture of the \( \psi \) for the non-bonding electrons on TOP of the structure
c) show that you understand the meaning of the hybridization assignment by making a small table 
that summarizes all of the valence hybrid (and any unhybridized) atomic orbitals associated with 
this carbon atom, and state how they are used (e.g. used to make a sigma bond to the chlorine, I 
know there is no chlorine in the structure, this is just to show you what do to)

\[ \text{d)} \]

give the approximate C-C-H bond angle indicated with the arrow, assign the geometry around 
the circled carbon 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".

there are 3 domains of electrons around the carbon, VSEPR requires a trigonal planar-like 
geometry to minimize the total energy of the electrons, because the carbon only has 2 atoms 
attached to it and the position of the electrons cannot be determined with certainty, the geometry 
can only be defined as bent