Name: Molly Qular Orbital  
Please use a non-red pen. Answer questions in the provided space. If you write any answers on the back of the page, indicate this on the front of that page. Points appear in parentheses ( ). Good Luck!

<table>
<thead>
<tr>
<th>Question</th>
<th>Points</th>
<th>Max. Points</th>
<th>Points Earned</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>(4 + 3) + 8</td>
<td>= 15</td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>6 + 2 + (3 + 6) + 3</td>
<td>= 20</td>
<td></td>
</tr>
<tr>
<td>3.</td>
<td>(4 + 4) + 3 + 3 + 2 + 4</td>
<td>= 20</td>
<td></td>
</tr>
<tr>
<td>4.</td>
<td>3 + 6 + 3 + 3</td>
<td>= 15</td>
<td></td>
</tr>
<tr>
<td>5.</td>
<td>6 + 3 + 3 + 3 + 3</td>
<td>= 18</td>
<td></td>
</tr>
<tr>
<td>6.</td>
<td>3 + 3 + 3 + 3</td>
<td>= 12</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>= 100</td>
<td></td>
</tr>
</tbody>
</table>

1. (15) a. Arrange the following bonds in order of increasing ionic character from least ionic to most ionic. Classify each bond as pure covalent, polar covalent, or ionic. You may use Pauling’s Electronegativity Table to guide you. Add charges, full or partial, as required to describe the bond.

<table>
<thead>
<tr>
<th>Bond Classification:</th>
<th>+ -</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-N</td>
<td>(1) δ⁺-δ⁻</td>
</tr>
<tr>
<td>K-Cl</td>
<td>(2) δ⁺-δ⁻</td>
</tr>
<tr>
<td>Si-C</td>
<td>(3) δ⁺-δ⁻const</td>
</tr>
<tr>
<td>N-H</td>
<td>(4) δ⁻-δ⁺</td>
</tr>
<tr>
<td>C-S</td>
<td>(5)</td>
</tr>
<tr>
<td>C-Br</td>
<td>(6) δ⁺-δ⁻</td>
</tr>
</tbody>
</table>

Ordering (least ionic to most ionic) + any charges or partial charges:
(5) > (6) > (1) > (3) > (4) > (2)

3. b. For each of the species below determine the following:
   (1) The formal charge on the Boldface Central Atom. Show the Formal Charge calculation.
   (2) The molecular shape of the species, i.e. tetrahedral, pyramidal, bent, trigonal, or digonal.

   \[
   \begin{align*}
   \text{CH}_3 & \quad \text{(1) } F = +1 \\
   \text{CH}_3-\text{O}= & \quad \text{(2) Shape = trig-pyramidal} \\
   \text{CH}_3 & \quad \text{(1) } F = -1 \\
   \text{H} & \quad \text{(2) Shape = tetrahedral} \\
   \text{H} & \quad \text{(1) } F = -1 \\
   \text{D} & \quad \text{(2) Shape = trig-pyramidal} \\
   \end{align*}
   \]
2. (20) a. Draw the molecular orbital structure of the following molecule showing $\sigma$ and $\Pi$ bonds, atom hybridization, nonbonding electrons, and bond angles and shapes.

![Molecular structure image]

- $107^\circ$ = trigonal-pyramidal
- $109.5^\circ$ = tetrahedral, $sp^3$
- $120^\circ$ = $sp^2$, trigonal-planar
- $180^\circ$ = $sp$, digonal-linear

b. Determine the Index of Hydrogen Deficiency, $\Omega$, for molecules with the molecular formula, $C_5H_6O$. Show your calculation.

$$\Omega = 5 - \frac{6}{2} + 1 = 3$$

2

c. Draw a variety of structures for 6 isomers of $C_5H_6O$. Include a cis-trans pair. For the other 4 isomers locate and label the following functional groups: an aldehyde, a ketone, a cyclic compound, and an alkyne.

![Isomer structures image]

- (1) cis
- (2) trans
- (3)
- (4)
- (5)
- (6)

6 Other isomers are possible.

d. Write a pair of resonance structures for the nitrite ion, $NO_2^-$.

![Resonance structures image]
3. (20) a. Name the following molecules according to IUPAC nomenclature.

(1) cis-1-chloro-6-isopropyl-3-methoxy-7-methyl-4-nonen-2-one

(2) \( t \)-butyl 6,7-dibromo-2-octynoate

b. Write the structure for: 4,4-dimethyl-2-cyclohexen-1-ol.

c. (1) Complete the following reaction showing the structure of the product.

(2) The name of the Corey-Posner, Whitesides-House product is:
   (a) 3,6-Dimethylheptane  (b) 3,5-Dimethylheptane  (c) 3,4-Dimethylheptane
   * (d) 2,5-Dimethylheptane  (e) 2,6-Dimethylheptane

d. Arrange the following bases in decreasing order of basicity (strongest to weakest base).
   (1) \( \text{CH}_3\text{C}^-\text{O}^- \)  (2) \( \text{CH}_3\text{C}≡\text{C}:^- \)  (3) \( \text{CH}_3\text{CH}_2::^- \)  (4) \( \text{N}(\text{CH}_3)_2^- \)  (5) \( \text{OC}(\text{CH}_3)_3^- \)

   (3) > (4) > (2) > (5) > (1)
4. (12)  
   a. Which compound below would have the lowest boiling point?

   ![Compounds Diagram](image)

   (1) (2) (3) (4) (5)

   b. Which of the following functional groups is **not** in atropine. Point out and label the location of the other functional groups.

   ![Atropine Structure](image)

   (1) Amine  (2) Ester  (3) Alcohol  (4) Ketone  (5) Benzene ring

   b. Fill in the missing reagents.

   ![Reaction Diagram](image)

   (1) cis-1,4-Di-tert-butylcyclohexane  (2) trans-1,4-Di-tert-butylcyclohexane

   (3) cis-1,3-Di-tert-butylcyclohexane  (4) trans-1,2-Di-tert-butylcyclohexane

   (5) None of these
5. (18)  a. Draw the structure of the following compound from its name and indicated stereochemistry. Show both possible conformers and calculate their relative stabilities ($\Delta G_{\text{str}}$) using the following table of $A$ values. Circle the more stable conformer and determine the number of kcal/mol by which it is more stable.

<table>
<thead>
<tr>
<th>Group:</th>
<th>-C(CH$_3$)$_3$</th>
<th>-COOH</th>
<th>-OH</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ kcal/mol</td>
<td>5.4</td>
<td>1.1</td>
<td>0.7</td>
</tr>
</tbody>
</table>

$\text{cis-3-hydroxy-4-t-butyl-1-carboxycyclohexane}$. 

\[
\Delta G_{\text{str}} = 0.7 + 1.1 = 1.8 \\
\Delta G_{\text{str}} = 5.4
\]

more stable by 3.6 kcal/mol

b. Which isomer would have the largest heat of combustion, ($\Delta H_{\text{combustion}}$)?

* (1) Propylcyclopropane  (2) Ethylcyclobutane  (3) Methylcyclopentane

(4) Cyclohexane  (5) Since they are all isomers, all would have the same $\Delta H_{\text{combustion}}$.

c. The least stable conformation of cyclohexane is the:

(1) boat  (2) twist boat  (3) chair  * (4) half-chair  (5) twist chair

d. Draw the structure of $\text{bicyclo[3.2.1]octane}$.

e. Using the sawhorse structures, draw the most stable conformer of 1,2-diphenylethane.
6. (12) a. Which acid-base reaction would not take place as written?

(1) \( \text{CH}_3\text{Li} + \text{HOH} \rightarrow \text{CH}_4 + \text{HOLi} \)

(2) \( \text{(CH}_3)_3\text{N} + \text{BF}_3 \rightarrow \text{(CH}_3)_3\text{NBF}_3 \)

(3) \( \text{CH}_3\text{CO}_2\text{H} + \text{CH}_3\text{ONa} \rightarrow \text{CH}_3\text{CO}_2\text{Na} + \text{CH}_3\text{OH} \)

* (4) \( \text{HCCH} + \text{NaOCH}_3 \rightarrow \text{HCN} + \text{HOCH}_3 \)

(5) \( \text{HC≡CNa} + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{HC≡C} + \text{NaOCH}_2\text{CH}_3 \)

b. Which of the following molecules would have a net dipole moment. Note all that pertain.

(1) \( \text{CBr}_4 \)

* (2) \( \text{CH}_2\text{Br}_2 \)

* (3) \( \text{(CH}_3\text{CH}_2)_2\text{C≡O} \)

(4) \( \text{CO}_2 \)

* (5) \( \text{H-C≡N} \)

\( \text{c. Check which of the acids below would have the strongest conjugate base? Write the structure of that base. Circle which of the acids below would have the weakest conjugate base. Write that base below.} \)

(1) \( \text{CH}_3\text{COOH} \) acetic acid \( K_a = 1.8 \times 10^{-05} \)

(2) \( \text{C}_6\text{H}_6 \) benzene \( K_a = 10^{-43} \)

(3) \( \text{H}_2\text{O} \) water \( K_a = 1.8 \times 10^{-16} \)

(4) \( \text{C}_6\text{H}_{12} \) cyclohexane \( K_a = 10^{-52} \)

(5) \( \text{(CH}_3)_3\text{CCOH} \) \( t \)-butyl alcohol \( K_a = 10^{-18} \)

(6) \( \text{CF}_3\text{COOH} \) trifluoracetic acid \( K_a = 1.0 \)

\( \text{strongest conjugate base} \quad \text{weakest conjugate base} \)

\( \text{O} \quad \text{CF}_3\text{C}--\text{O} \)

\( \text{d. Give 2 reasons why trichloroacetic acid is a stronger acid than acetic acid.} \)

(1) Electronegative Cl’s make it easier for \( \text{H}^+ \) to escape.

(2) Electronegative Cl’s stabilize carboxylate anion.

(3) Electronegative Cl’s in stabilizing carboxylate anion mean that not as much hydration of anion is needed so entropy (ordering) requirement is decreased.