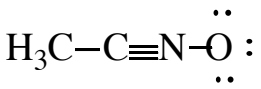
**1. Multiple Choice Questions (15 points)**
Please **circle the best answer** to each question. Lone pairs are generally not shown.

**(i)** The formal charges on the nitrogen and oxygen atoms in the structure



are, respectively:
(A) 0, 0 **(B) +1, -1** (C) –1, +1 (D) 0, -1

**(ii)** Do these two structures have the same molecular geometry?

(A) Yes, both are linear.
(B) Yes, both are bent.
**(C) No; the first is linear and the second is bent.**
(D) No; the first is bent and the second is linear.

**(iii)** How many π bonds are there in the molecule $H_2C{=}CH{-}C{\equiv}N$?
(A) two **(B) three** (C) four (D) five

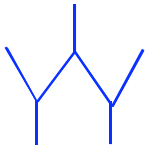
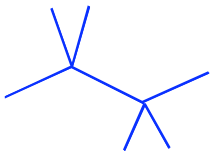
**(iv)** Select the <u>correct</u> statement about the $H_3C{-}O{-}CH_3$ molecule.
(A) It is nonpolar.
(B) The C-O-C bond angle is 180°.
(C) It is a stereoisomer of ethanol, $CH_3CH_2OH$.
**(D) It is a constitutional isomer of ethanol, $CH_3CH_2OH$.**

**(v)** Cycloalkanes are characterized by the general molecular formula:
(A) $C_nH_{2n-2}$
(B) $C_nH_{2n+2}$
**(C) $C_nH_{2n}$**
(D) $C_nH_{2n+4}$

*Points earned on this page* ___

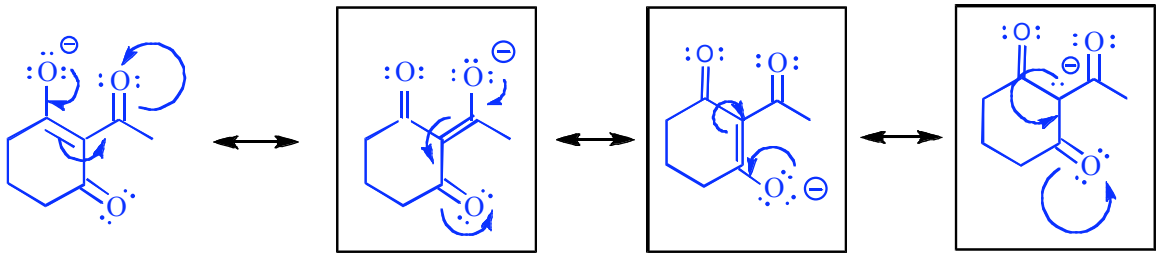
2. (12 points)

Using **bond-line formulas**, draw ONLY the constitutional isomers of $C_8H_{18}$ that are described below and write the corresponding IUPAC name.

| | **Bond-line formula** | Correct IUPAC name |
|---|---|---|
| (A) a substituted hexane |  | 3, 3-dimethylhexane |
| (B) a substituted pentane |  | 2, 3, 4-trimethylpentane |
| (C) a substituted butane |  | 2, 2, 3, 3-tetramethylbutane |

3. (9 points)

Draw three other stable resonance contributors for this anion, showing all non-zero formal charges. Clearly show all lone pairs and appropriate curved arrow notation to interconvert the contributing structures.



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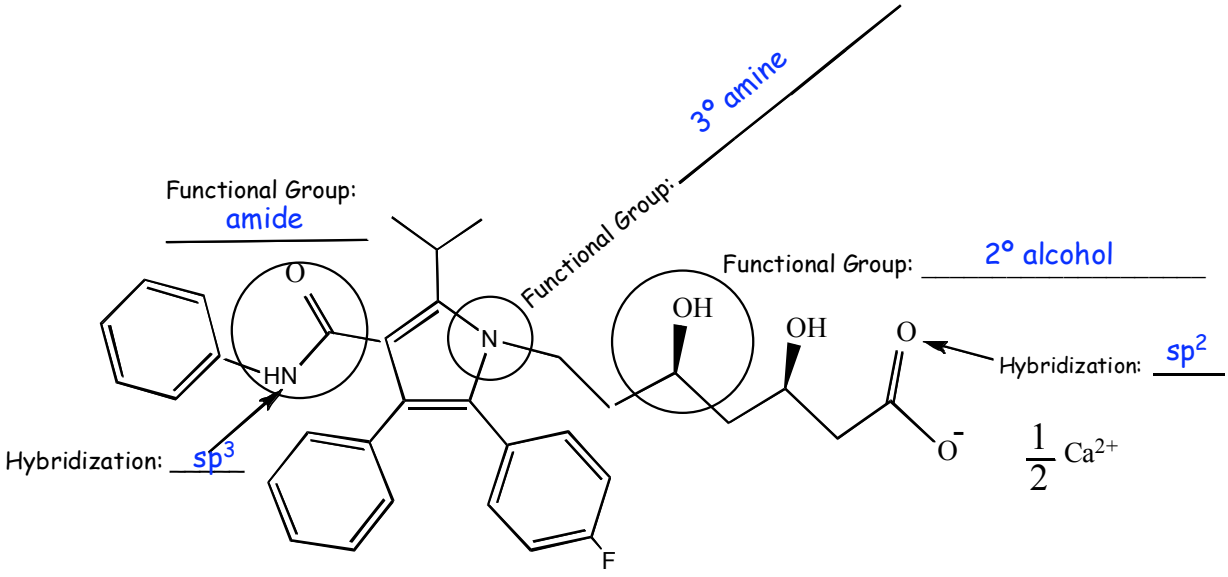
4. (10 points) Statin drugs lower cholesterol by inhibiting the enzyme 3-hydroxy-3-methylglutaryl coenzyme A reductase that is required for the biosynthesis of mevalonic acid (a precursor to cholesterol). Name all the circled functional groups in the spaces provided and indicate the hybridization of the atoms that the arrows point to in the structure for Atorvastatin calcium (marketed as Lipitor). If an alcohol or amine group is present, please identify it as primary, secondary, or tertiary. NOTE: Lone pairs are not shown.




Circle the best answer possible.

(A) The hybridization of the carbon atom in the carboxylic acid functional group is:

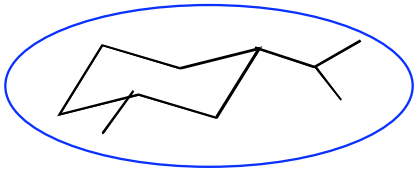
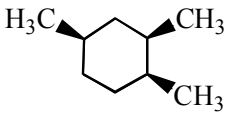
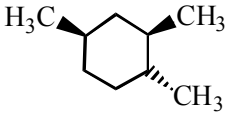
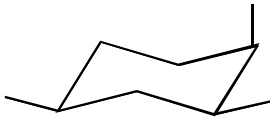
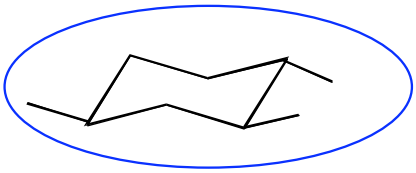
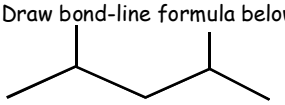
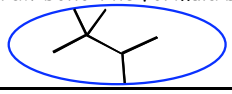
$sp^3$ (circled: $sp^2$) sp

(B) An _____ is a carboxylic acid derivative.

ether aldehyde (circled: ester)

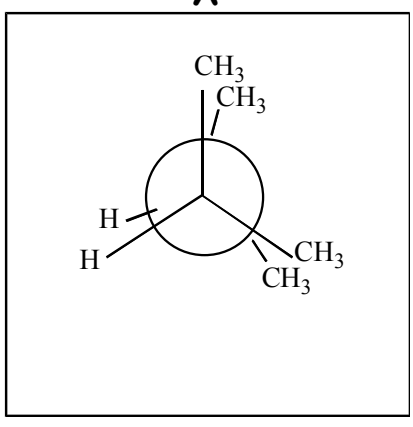
*Points earned on this page* ___

5. (15 points) Draw a structure for each compound as described in the table below. Then, **circle the more stable compound in each pair.**

| (A) *cis*-1-isopropyl-3-methylcyclohexane | or | *trans*-1-isopropyl-3-methylcyclohexane |
|---|---|---|
| Draw most stable chair conformation below:  | | Draw most stable chair conformation below:  |
| (B)  | or |  |
| Draw most stable chair conformation below:  | | Draw most stable chair conformation below:  |
| (C) 2, 4-Dimethylpentane | or | 2, 2, 3-trimethylbutane |
| Draw bond-line formula below:  | | Draw bond-line formula below:  |

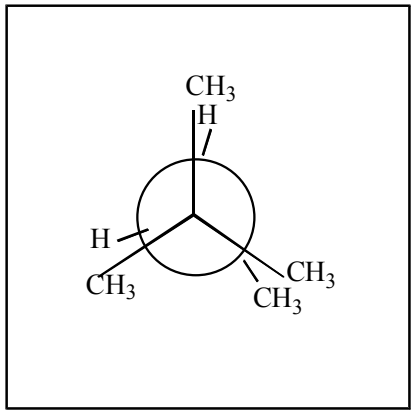
6. (6 points) Draw Newman projections looking down the C2-C3 bond of 2, 3-dimethylbutane for (A) the least stable eclipsed conformation and (B) the relatively more stable eclipsed conformation .

**A**




CH3
CH3

**B**

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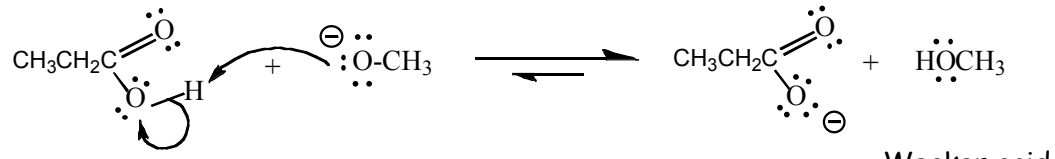
7. (15 points)
(A) Identify each statement as true(**T**) or false(**F**).

**F** (i) $CHCl_2COOH$ is a weaker acid than $Cl_2CHCH_2COOH$.

**T** (ii) The t-butoxide ion, $(CH_3)_3CO^-$, is a stronger base than the hydroxide ion.

**F** (iii) Phenol, $C_6H_5OH$, is a stronger acid than $CH_3COOH$.

7(B) Draw an arrow-pushing mechanism for the acid-base reaction between propanoic acid, $CH_3CH_2COOH$, $pK_a$ = 4.9, and the methoxide ion, $CH_3O^-$. **Draw the structures of the products.** The $pK_a$ of methanol, $CH_3OH$, is 15.2. Clearly indicate **on the arrow(s)** which side of the reaction is favored at equilibrium and explain your reasoning in one sentence. Show all lone pairs and formal charges throughout your mechanism.




Stronger acid Weaker acid

Equilibrium favors formation of weaker acid and weaker base from reaction of stronger acid and stronger base OR equilibrium favors direction of higher $pK_a$.

7(C) When $NH_3$ reacts with water:
(i) the attacking electrons are in a(n) nonbonding molecular orbital
(choices are s, p, $sp^2$, $sp^3$, nonbonding, N-H $\sigma$, N-H $\sigma^*$),
and
(ii) the empty orbital into which the electrons are transferred is a(an) O-H $\sigma^*$ molecular orbital.
(Choices are s, p, $sp^2$, $sp^3$, O-H $\sigma$, O-H $\sigma^*$).

*Points earned on this page* ___

8. (18 points) Heats of combustion data are useful in comparing relative stabilities of organic compounds.

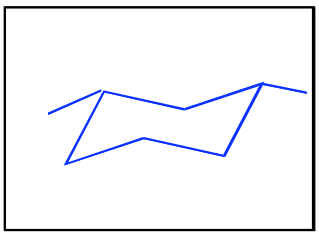
(i) Arrange these isomeric cycloalkanes in increasing order of $|\Delta H_{comb}|$. Write the names of the compounds in the boxes below.

*cis*-1,2-dimethylcyclopropane, cyclopentane, and methylcyclobutane

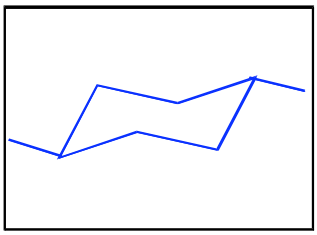
increasing order of $|\Delta H_{comb}|$

| cyclopentane | < | methylcyclobutane | < | *cis*-1,2-dimethyl cyclopropane |
|---|---|---|---|---|
| most stable<br>lowest $\Delta H_{comb}$ | | | | least stable<br>highest $\Delta H_{comb}$ |

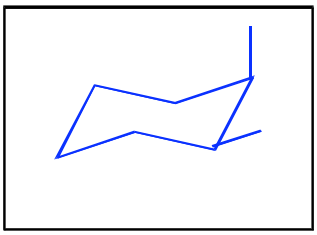
(ii) When comparing $|\Delta H_{comb}|$ for the isomeric dimethylcyclohexanes, the values ranged from 5212 kJ/mol to 5223 kJ/mol. Two stereoisomers have the value of 5212 kJ/mol while only one stereoisomer has the value of 5223 kJ/mol. Draw the most stable chair comformations for these stereoisomers in the appropriate boxes.



$|\Delta H_{comb}|$ = 5212 kJ/mol



$|\Delta H_{comb}|$ = 5212 kJ/mol



$|\Delta H_{comb}|$ = 5223 kJ/mol

The isomeric dimethylcyclohexanes are 1,1-dimethylcyclohexane, *cis*- and *trans*-1, 2-dimethylcyclohexane, *cis*- and *trans*-1, 3-dimethylcyclohexane, and *cis*- and *trans*-1,4-dimethylcyclohexane. Except for the first compound, the other six are three pairs of stereoisomers. Of all these stereoisomers, the most stable equatorial-equatorial conformations are present in *cis*-1, 3 and *trans*-1, 4 compounds. Both *cis*- and *trans*-1, 2 compounds have relatively higher heats of combustion than the other *cis*-(1, 3- and 1,4-) and *trans*-(1, 3- and 1,4-)isomers. Please refer to assigned homework problem 3.32; there are gauche interactions in the 1, 2-isomers.

*Points earned on this page* ___