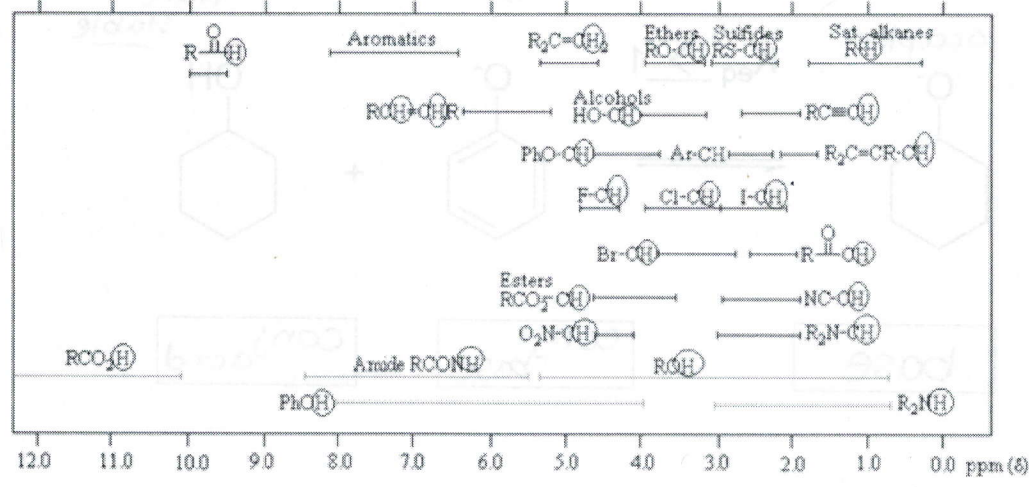


**Periodic Table of the Elements**

**Typical Infrared Stretching Frequencies**

Functional Group	Bond	Stretching, $\text{cm}^{-1}$	Intensity
alcohol	O-H	3650 - 3200	strong; broad (H-bonded)
amine, amide	N-H	3500 - 3200	medium; often broad
alkyne	$\equiv\text{C-H}$	3340 - 3250	strong
aryl, vinyl	$\text{sp}^2\text{C-H}$	3100 - 3000	weak to strong
carboxylic acid	O-H	3000 - 2500	strong; often very broad
alkyl	$\text{sp}^3\text{C-H}$	2960 - 2850	variable; usually strong
aldehyde	$\text{sp}^2\text{C-H}$	~2900 and ~2700	medium; 2 bands
nitrile	$\text{C}\equiv\text{N}$	2260 - 2220	weak to strong
alkyne	$\text{C}\equiv\text{C}$	2260 - 2000	weak to strong
ester	$\text{C}=\text{O}$	1750 - 1735	strong
aldehyde	$\text{C}=\text{O}$	1740 - 1720	strong
ketone	$\text{C}=\text{O}$	1750 - 1705	strong
carboxylic acid	$\text{C}=\text{O}$	1725 - 1700	strong
amide	$\text{C}=\text{O}$	1690 - 1650	strong
alkene	$\text{C}=\text{C}$	1680 - 1620	weak to strong



**Typical Carbon NMR Chemical Shifts (ppm)**  
( $\text{CH}_3$ )<sub>4</sub>Si = TMS = 0.00 ppm

RCH <sub>3</sub>	0 - 40	RCH <sub>2</sub> Cl	35 - 80	benzene ring $\text{sp}^2\text{C}$	110 - 160
RCH <sub>2</sub> R	15 - 55	R <sub>3</sub> COH	40 - 80	C=O ester	160 - 180
R <sub>3</sub> CH	20 - 60	R <sub>3</sub> COR	40 - 80	C=O amide	165 - 180
RCH <sub>2</sub> I	0 - 40	RC $\equiv$ CR	65 - 85	C=O carboxylic acid	175 - 185
RCH <sub>2</sub> Br	25 - 65	R <sub>2</sub> C=CR <sub>2</sub>	100 - 150	C=O aldehyde, ketone	180 - 220

I pledge that I will do this test by myself and I will not give or receive help from anybody. I will not break the trust of Dr. Castillo by committing any form of fraud, by searching for the answers on the internet or by uploading the questions of this test on any website in order to get the answers. I understand that Dr. Castillo reserves the right to reach out to me and do an oral evaluation of the topics of this exam when and how she sees fit. I recognize there will be consequences, such as failing this test, if there is any form of cheating and that it will be reported to the Dean of Students for further academic actions. This test is a copyrighted material of the course instructor. Unauthorized sharing, dissemination or reproduction of any part of the exam in any form without explicit written permission from the instructor is a direct violation of the UCLA Conduct Code 102.23.

x Christina Kilkeary

## Final-Dec 12th

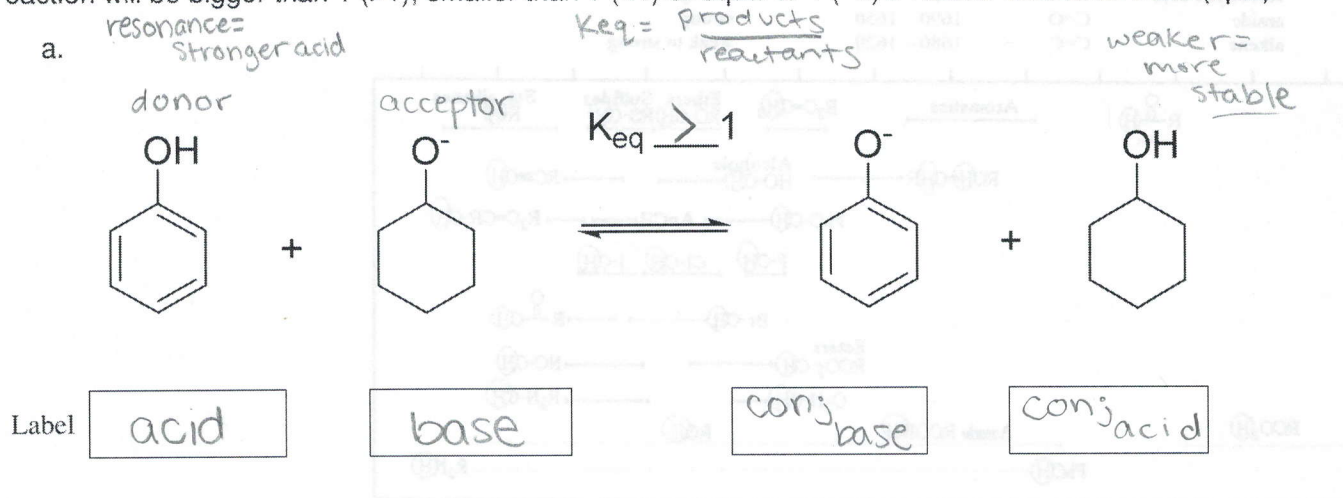
Chem14C-Fall2020

Prof. Castillo

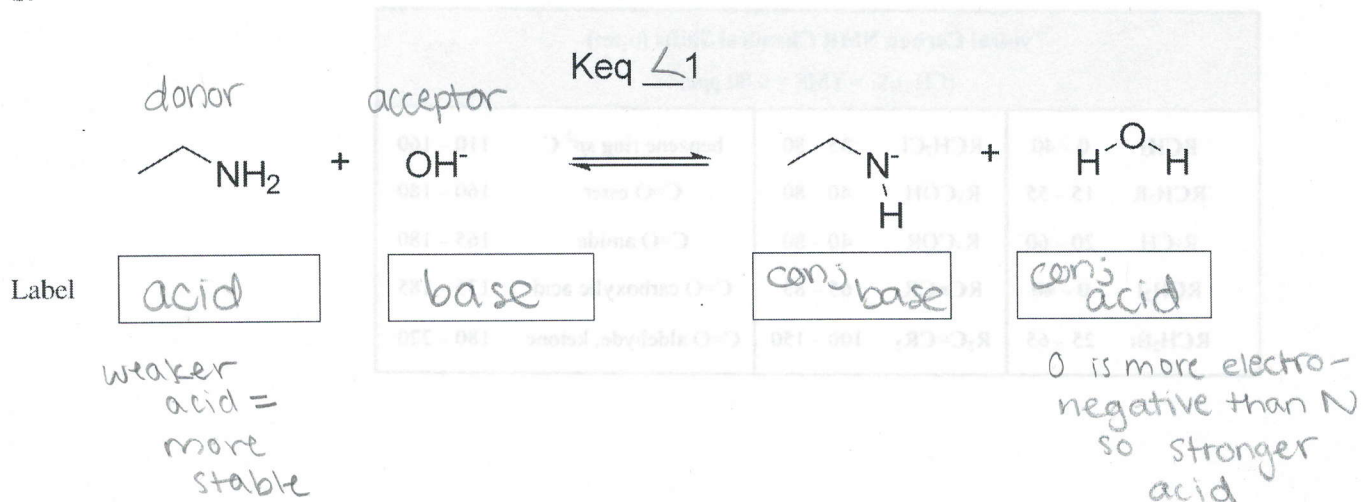
Name: Christina Kilkeary

ID: 605416454

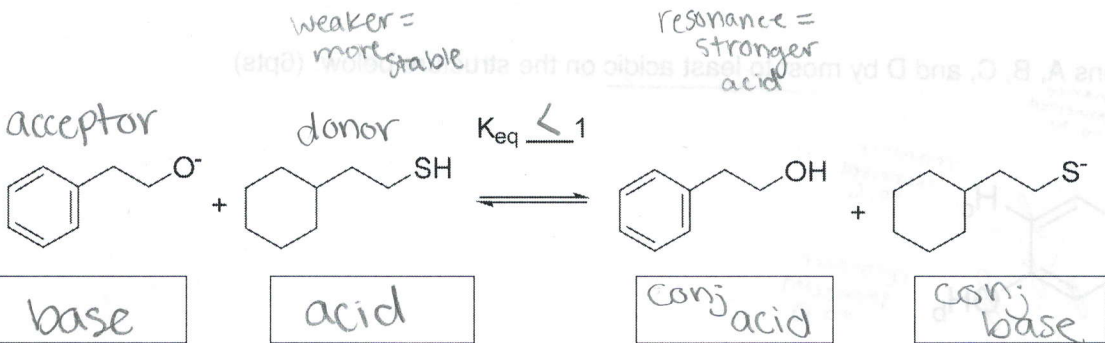
1. For the following reactions, label the "acid" or "base" on the left side of the reaction and "conjugate acid" or "conjugate base" on the right side of the reaction. Additionally, estimate if equilibrium constant ( $K_{eq}$ ) for each reaction will be bigger than 1 ( $>1$ ), smaller than 1 ( $<1$ ) or equal to 1 ( $=1$ ) if neither side is favored. (8pts)



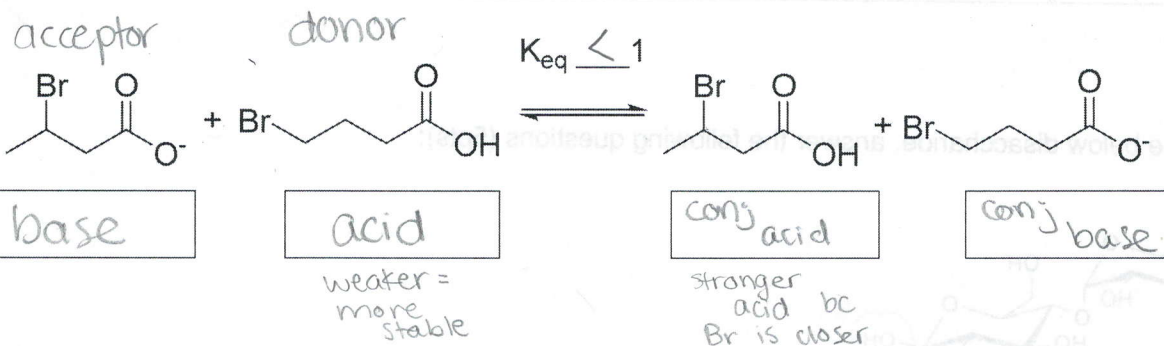
b.



c.

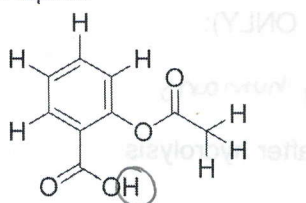


d.

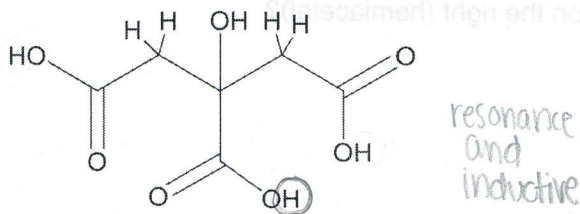


2. Below are structures for common drugs or household chemicals. Circle the most acidic hydrogen for each molecule, or multiple if they are equivalent. (5pts)

a. Aspirin



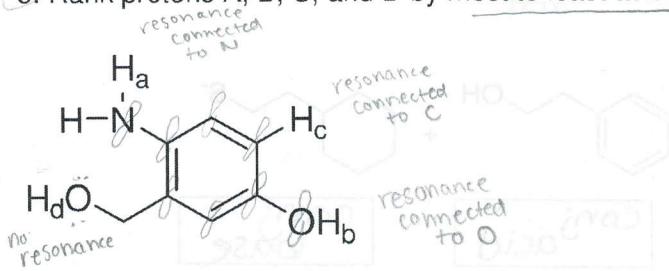
b. Citric acid



c. Tenormin

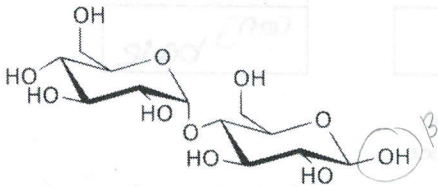


3. Rank protons A, B, C, and D by most to least acidic on the structure below. (6pts)



Most acidic	2 <sup>nd</sup> most acidic	3 <sup>rd</sup> most acidic	Least acidic
B	A	C	D

4. For the below disaccharide, answer the following questions (5pts):



a) What is the name of this disaccharide? Maltose

b) Is this disaccharide easily digested by human? Circle one:  yes or no

c) Provide explanation for your answer from question b (ONE SENTENCE ONLY):

α-linkage (alpha linkage) makes it easily digested by humans

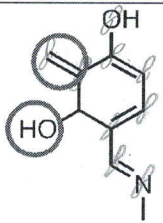
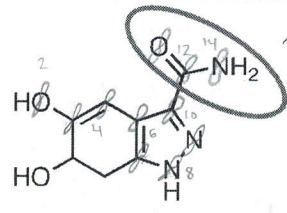

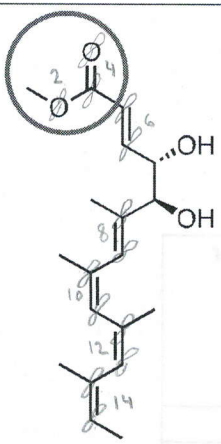
d) Name the two monosaccharide that this disaccharide would break into after hydrolysis

glucose and glucose

e) What is the configuration of the monosaccharide on the right (hemiacetal)?

Circle one:  α or  β

5. Fill out the table with the required information (5pts)

Structure	Number of atoms in the <b>longest</b> conjugation chain	Number of $sp^2$ hybridized atoms	Number of pi electrons	Indicate the name of the <b>circled functional groups</b>
	8	9	10	alkene alcohol
	11	11	14	amide
	5	5	4	alkene
	8	13	14	ester

↑ conjugation means ↓ HOMO LUMO

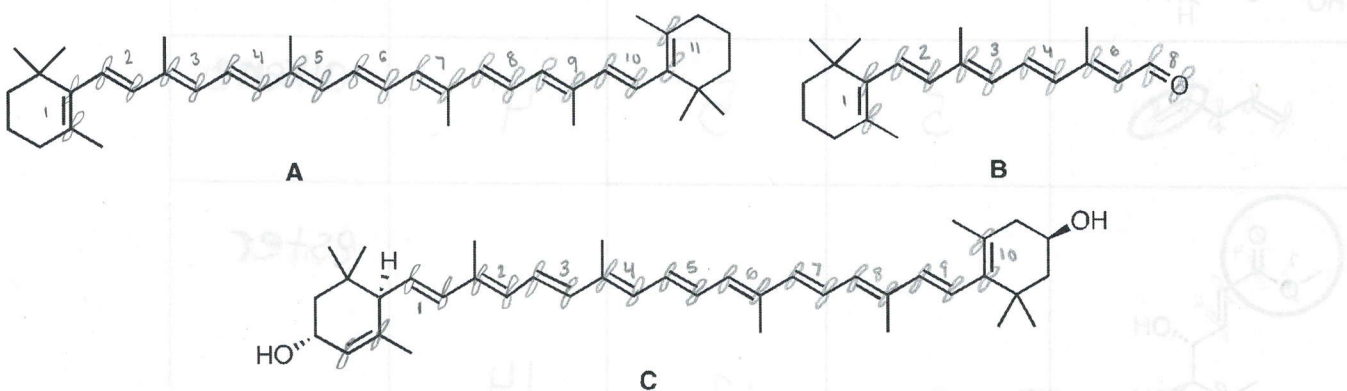
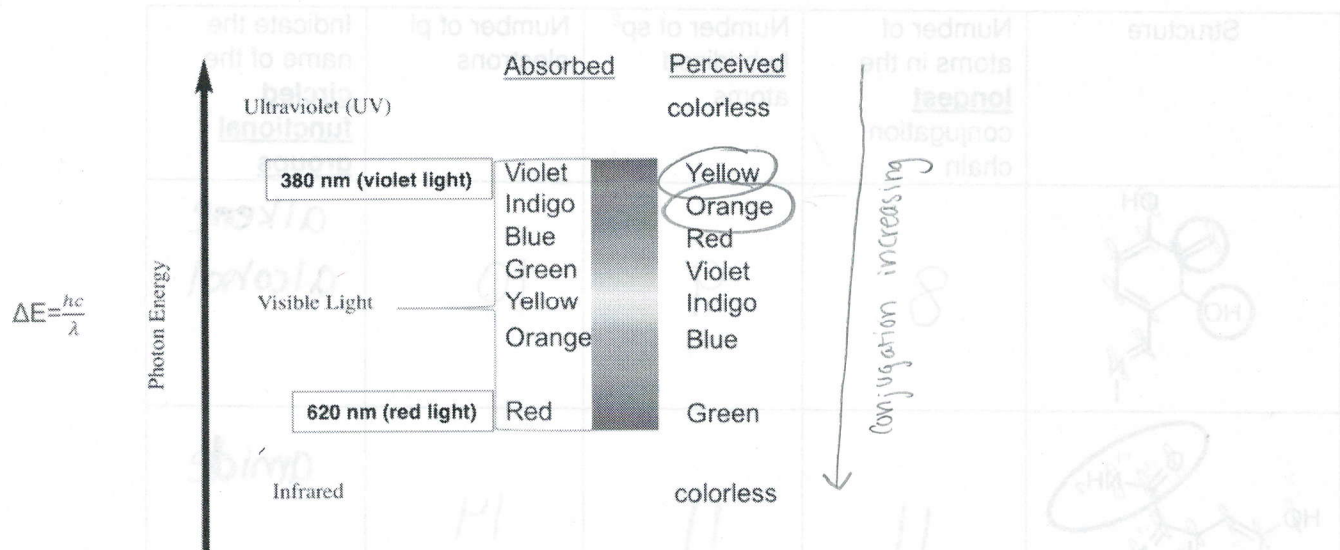
6. (5pts) Use the relationship that we learned in class between conjugated molecules,  $\Delta E$  HOMO  $\rightarrow$  LUMO gap, the energy of photon absorbed, color of photon absorbed and non-absorbed photons perceived color to fill out the blanks in the following questions.

First, indicate the number of **conjugated pi bonds** present in each following molecule;

Second, based on the relationship between conjugation and  $\Delta E$ , indicate which molecule has the highest  $\Delta E$  (please label with 1), which one has the intermediate  $\Delta E$  (please label with 2), and which one has the lowest  $\Delta E$  (please label with 3);

Finally, for molecule **A and C**, indicate which molecule is **perceived** as orange color, and which molecule is **perceived** as yellow color. An information about the absorption spectrum of visible light and corresponding perceived color is given below as well.

5. Fill out the table with the required information (5pts)



Structure	Indicate the number of <b>conjugated</b> pi bonds	Rank the energy gap difference $\Delta E$ of these molecules from highest (1) to smallest (3)	<b>Perceived</b> color
A	11	3	orange
B	8	1	<del>colorless</del>
C	10	2	yellow

8. (5pts) Use the relationship that we learned in class between conjugated molecules,  $\Delta E$  HOMO-LUMO gap, the energy of photon absorbed, color of photon absorbed and non-absorbed photons perceived color to fill out the blanks in the following questions.

First, indicate the number of **conjugated pi bonds** present in each following molecule.

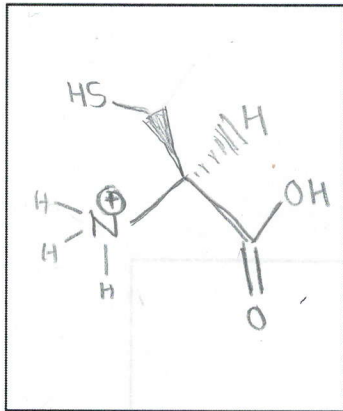
Second, based on the relationship between conjugation and  $\Delta E$ , indicate which molecule has the highest  $\Delta E$  (please label with 1), which one has the intermediate  $\Delta E$  (please label with 2), and which one has the lowest  $\Delta E$  (please label with 3).

Finally, for molecule A and C, indicate which molecule is perceived as orange color, and which molecule is perceived as yellow color. An information about the absorption spectrum of visible light and corresponding perceived color is given below as well.

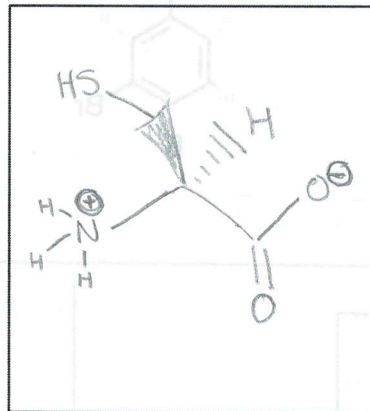
conjugation rises as HOMO, LUMO gap falls

7. Draw the structure for serine at pH 1.5, 7, and 9 (5pts)

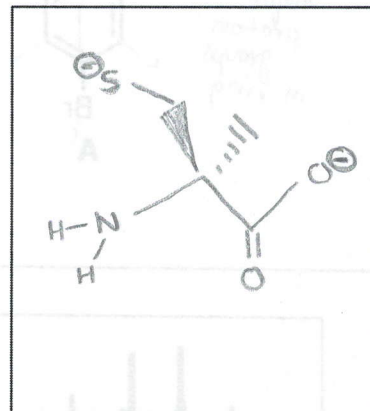
Cysteine R = CH<sub>2</sub>SH, pK<sub>a</sub> α-COOH = 2.0, pK<sub>a</sub> α-NH<sub>3</sub><sup>+</sup> = 10.3, pK<sub>a</sub> of acidic function in R = 8.2



pH 1.5  
(+)

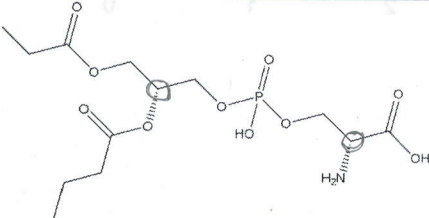
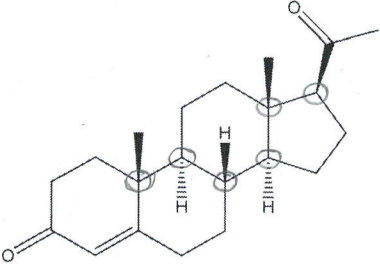
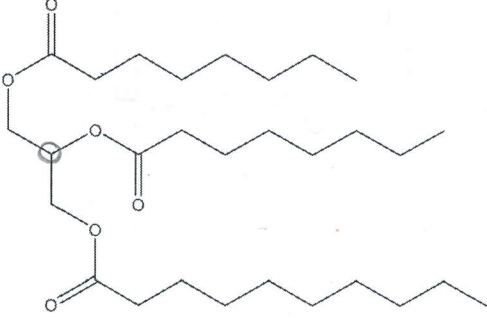


pH 7  
neutral

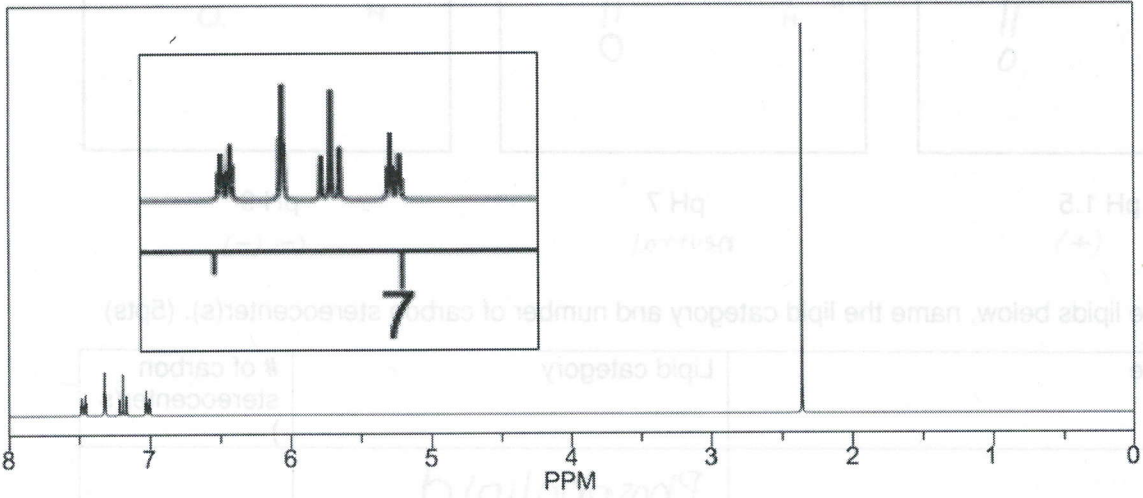
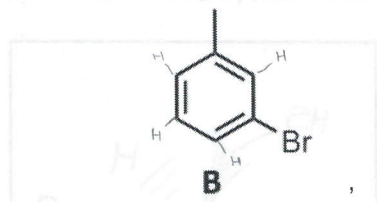
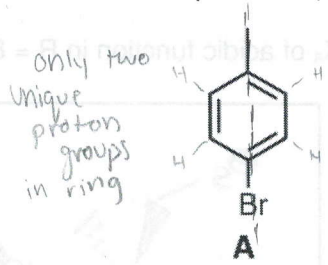


pH 9  
(-)(-)

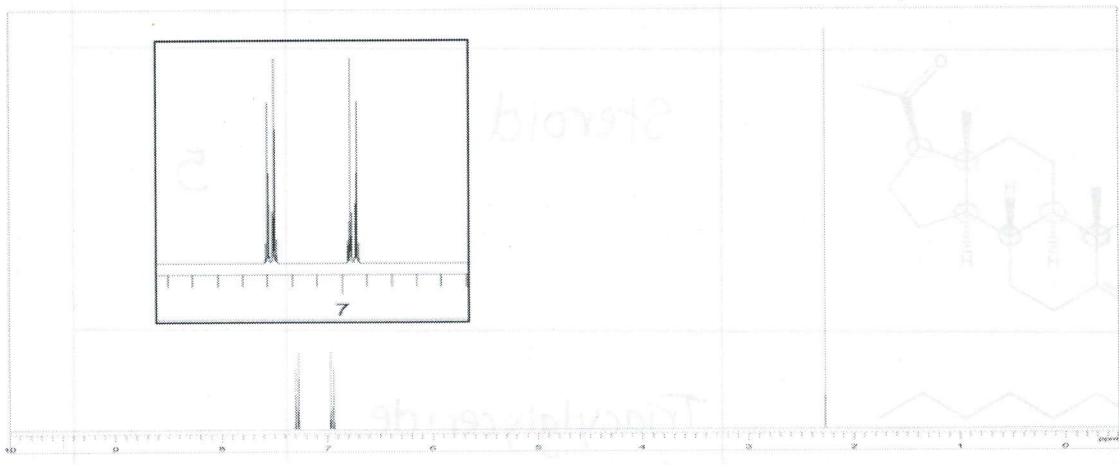
8. For the lipids below, name the lipid category and number of carbon stereocenter(s). (5pts)

Structure	Lipid category	# of carbon stereocenter(s)
	Phospholipid	2
	Steroid	5
	Triacylglyceride	1

9. Match each molecule to its spectrum. (5pts)



This spectrum belongs to molecule:  B



This spectrum belongs to molecule:  A



10. Predict the molecule using the following MS, IR, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra. (13pts)

**Mass spec:** m/z = 150 (100%), 151 (10.1%), 152 (0.2%)

**MS workspace.** Propose possible molecular formula with the information given from MS. Show all work to receive full credit.

$$\frac{10.1}{1.1} = 9 \text{ (carbons)}$$

Even # of Nitrogens

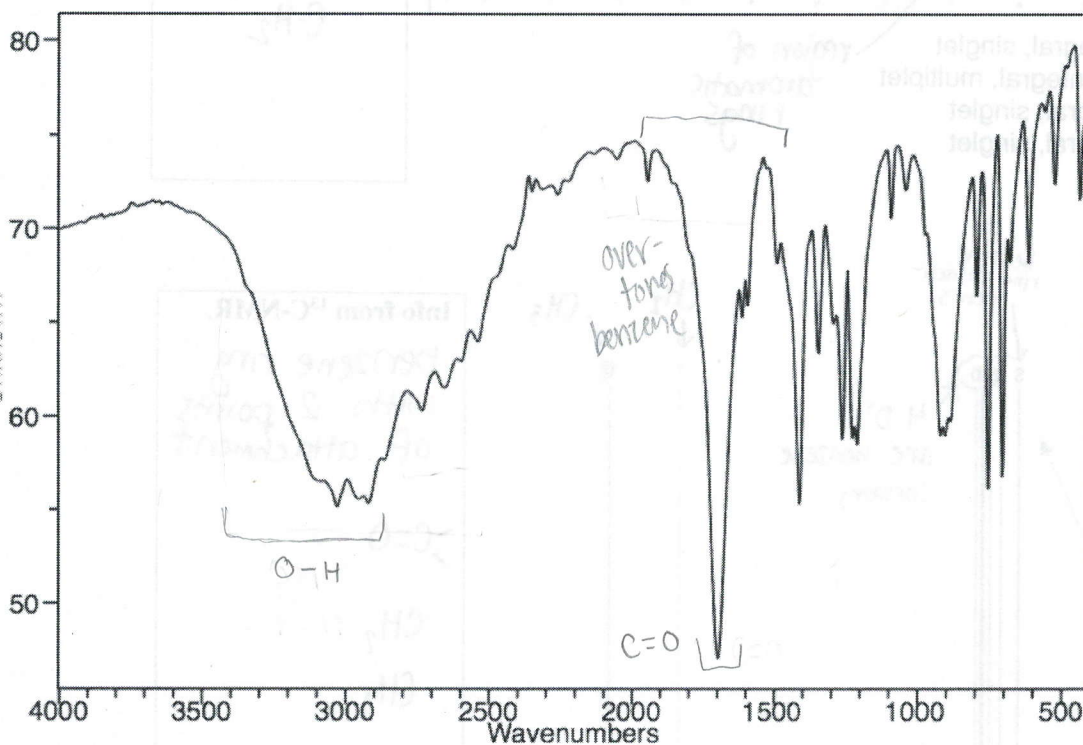
no halides

$$150 - (9 \cdot 12) = 42 \text{ amu left}$$

O	N	max H	amu left	formula
2	0	20	10	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ✓
0	2	22	14	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>

possible formulas

$$\text{max H formula} = 2C + N + 2$$



**IR workspace:** What functional groups are present? (Please provide the region in the IR with its respective bond type)

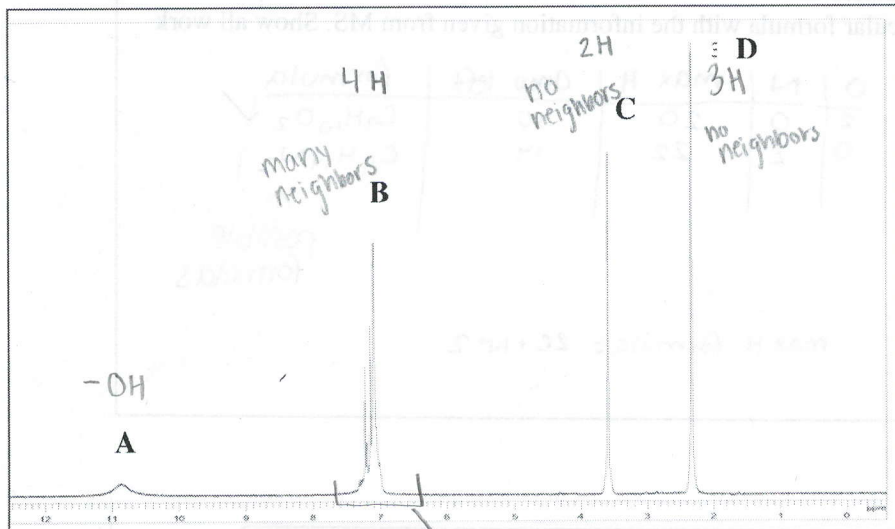
O-H and C=O are present and indicate carboxylic acid

weak overtones from 2000-1600 suggest benzene ring

(3500-3200 O-H) (1725-1700 C=O)  
(3000-2500 O-H)

What is the molecular formula?  $C_9H_{10}O_2$   
 Degrees of unsaturation: 5

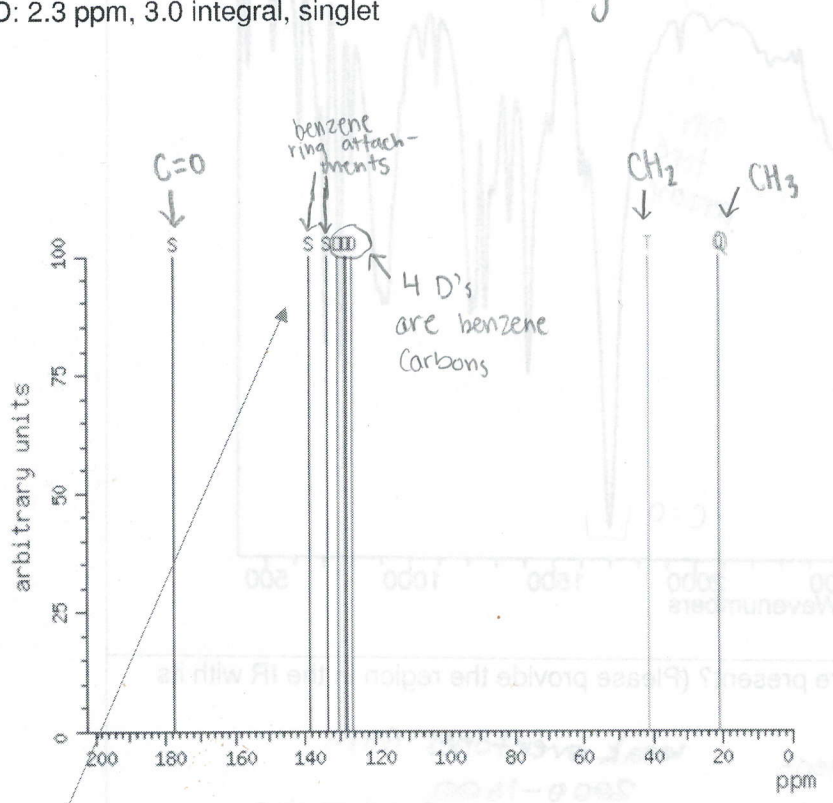
$DOU = C - \frac{H}{2} + \frac{N}{2} + 1$   
 $9 - 5 + 1 = 5$  DOU



**Info from NMR.**

A is OH  
 B is a benzene ring  
 C may be an isolated C-H<sub>2</sub>  
 D may be isolated CH<sub>3</sub>

A: 10.9 ppm, 1.0 integral, singlet  
 B: 7.3-7.0 ppm, 4.0 integral, multiplet  
 C: 3.6 ppm, 2.0 integral, singlet  
 D: 2.3 ppm, 3.0 integral, singlet

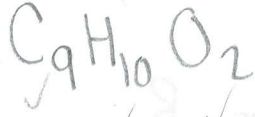


**Info from 13C-NMR.**

benzene ring with 2 points of attachment  
 C=O  
 CH<sub>2</sub>  
 CH<sub>3</sub>

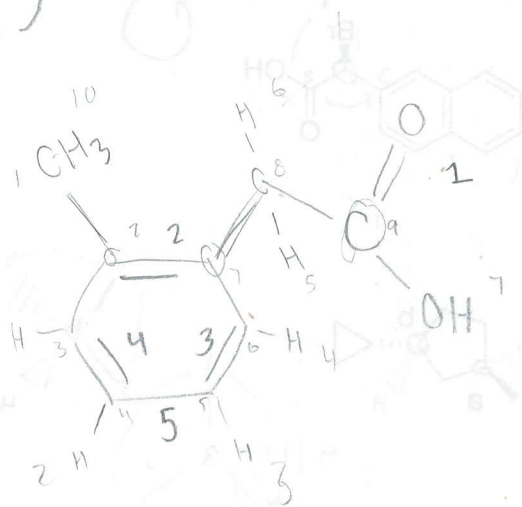
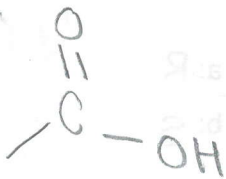
S S D D D D (6 signals)

Propose the structure of the molecule in the box to the right. Only one structure is graded. You may use this space to work out the problem. This space will not be graded

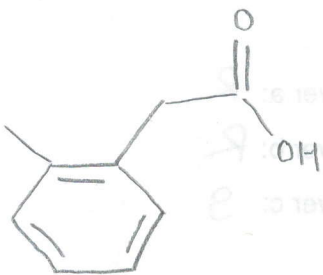


DOU = 5

pieces:

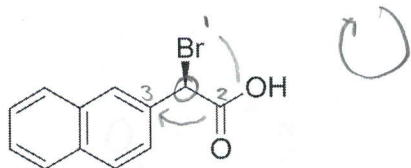


Proposed structure:



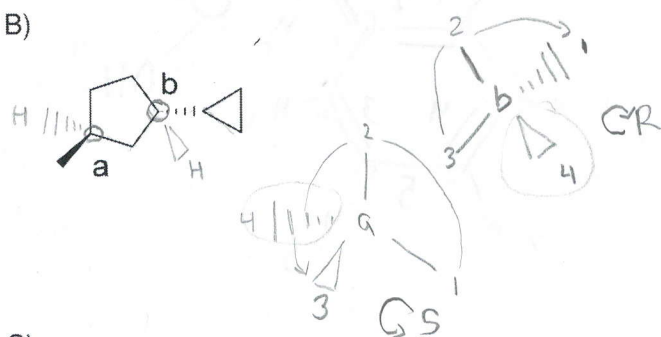
11. What is the absolute configuration (R/S) of the following centers? (10pts)

A)



Answer: R

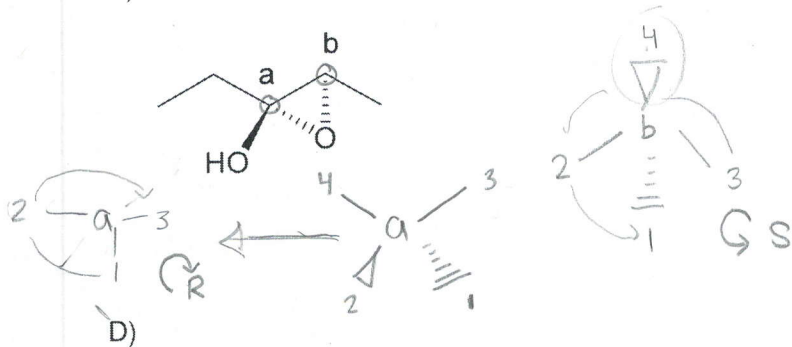
B)



Answer a: S

Answer b: R

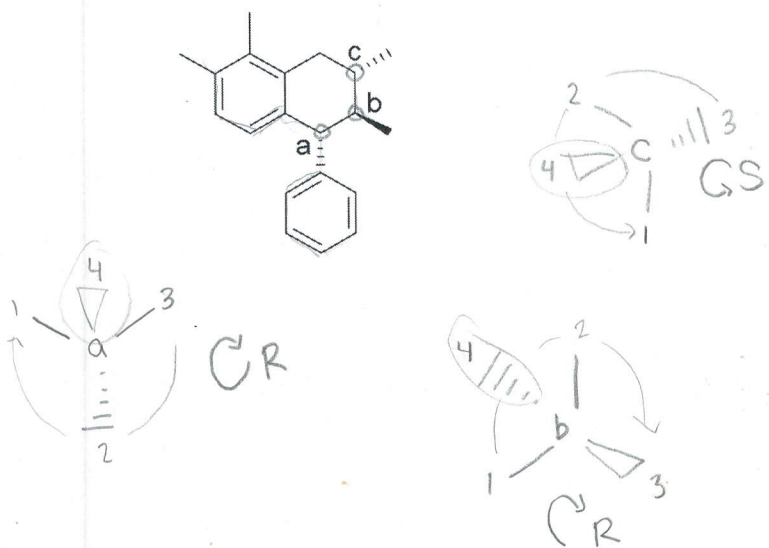
C)



Answer a: R

Answer b: S

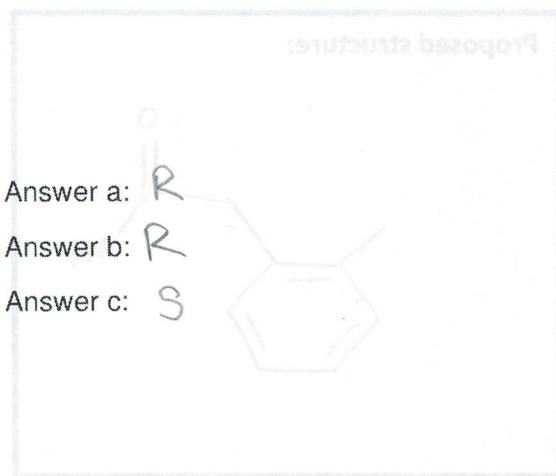
D)



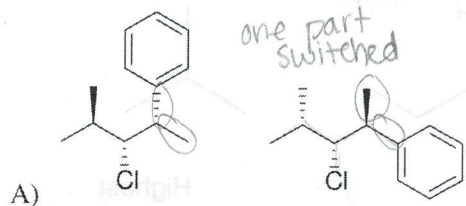
Answer a: R

Answer b: R

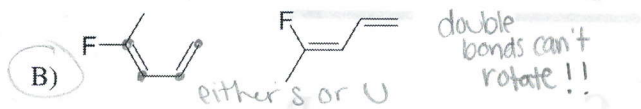
Answer c: S



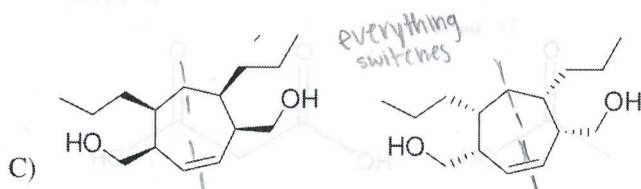
12. Indicate the relationship for the following pairs of compounds. Write **S** for same molecule, **E** for enantiomers, **D** for diastereomers, or **U** if the molecules are unrelated. (5pts)



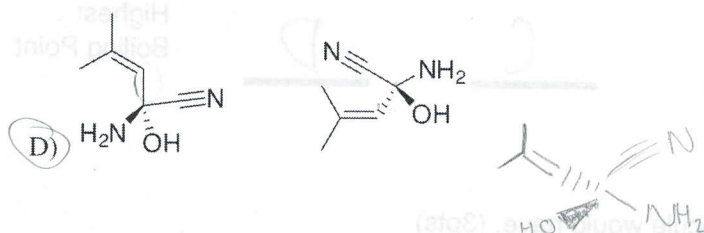
Answer: **D**



Answer: **U**



Answer: **E**

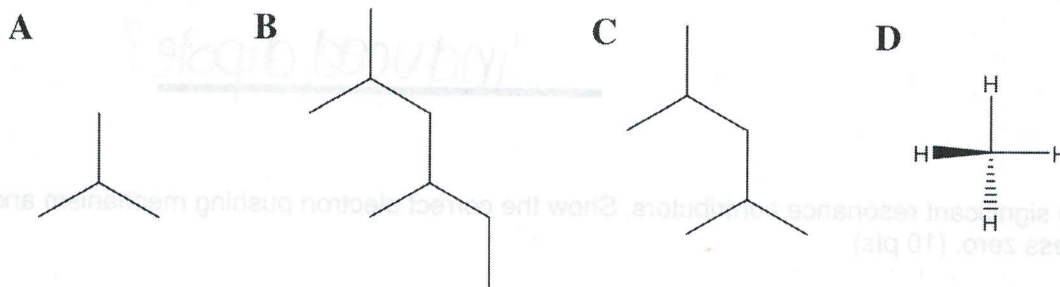


Answer: **S**

Which molecule from Q12 is a meso compound? Write the letter below.

Answer:   **C**  

13. Rank the following molecules in order of increasing boiling point value. (10pts)



Lowest Boiling Point

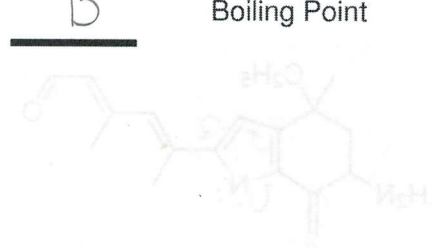
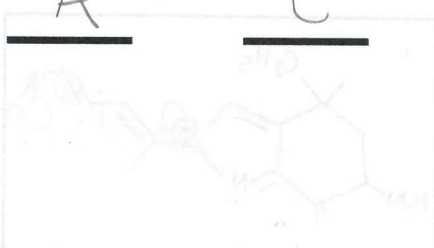
**D**

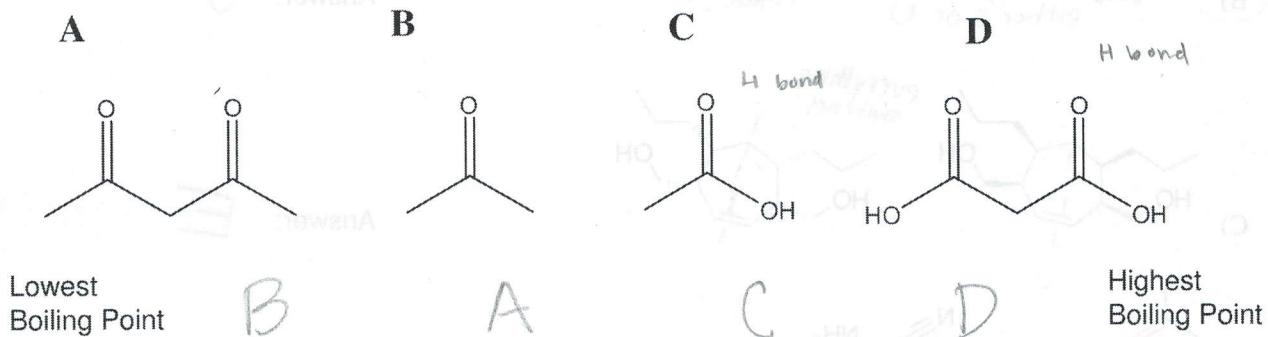
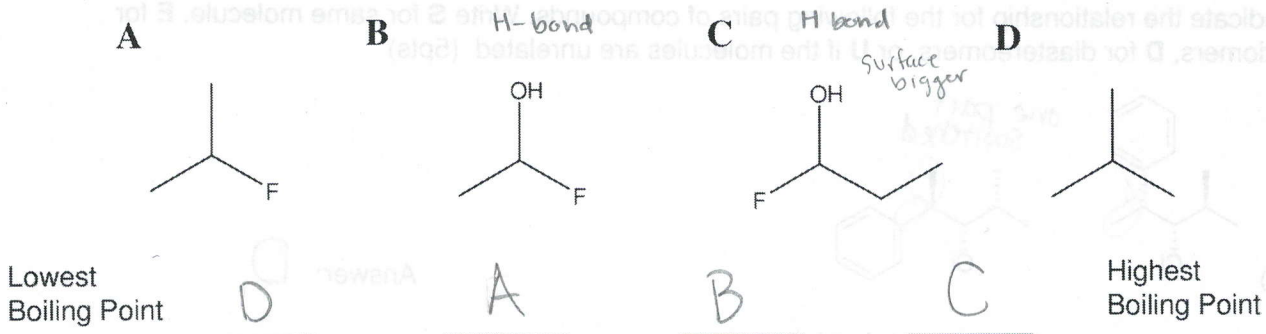
**A**

**C**

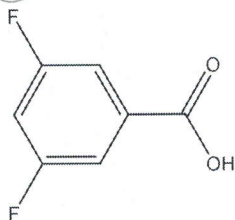
**B**

Highest Boiling Point





14. Name 4 intermolecular interactions that this molecule would have. (3pts)



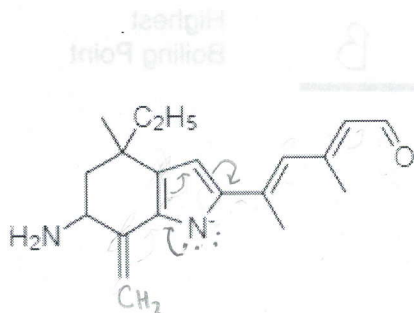
LDF

H-bond

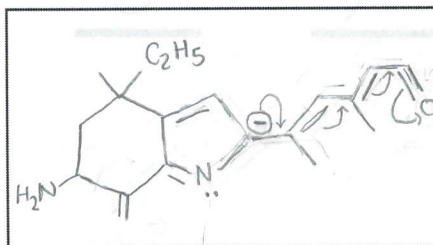
dipole-dipole

induced dipole?

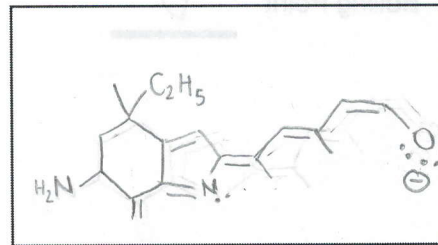
15. Draw two significant resonance contributors. Show the correct electron pushing mechanism and the formal charges, unless zero. (10 pts)



A



B



C

A- The best resonance contributor is C

$$4n+2 = 6$$

B- Has structure the given structure (A) an aromatic ring(s)? Y / N

C- Total number of electrons in p-orbitals ( $\pi$ -electrons) in the given structure (A): 14

D- How many chiral center in the given structure (A): 2

