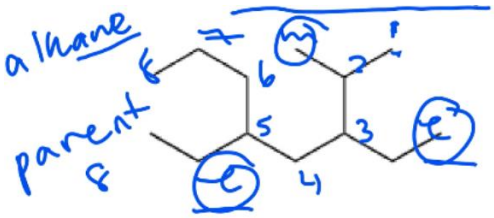
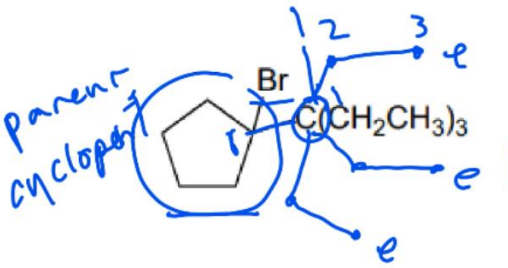
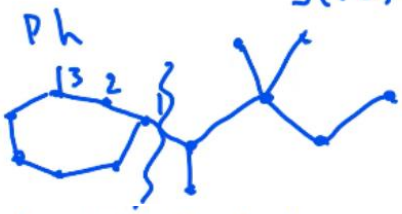
2A) Nomenclature (10 pts) Name each of the following compounds according to the IUPAC rules. Be sure to indicate stereochemistry, when appropriate. **You must show your work for full credit.**





2B) (5 pts) Draw 1-(1,2,2-trimethylbutyl)-3-phenylcycloheptane

3(1C)+4C=7C



2C) (4 pts) Calculate the degrees of unsaturation (DU or HDI) for the following compound. **Show your work for credit. No work = no credit.**

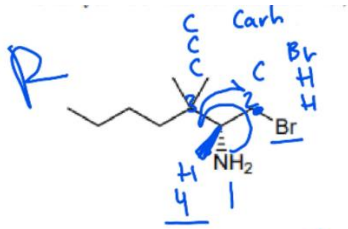
$C_7H_9BrO_2$ DU: 3 DU

$C_7H_{10} \rightarrow C_7H_{16}$ sat'd diff of 6H → 2H per 1° unsat

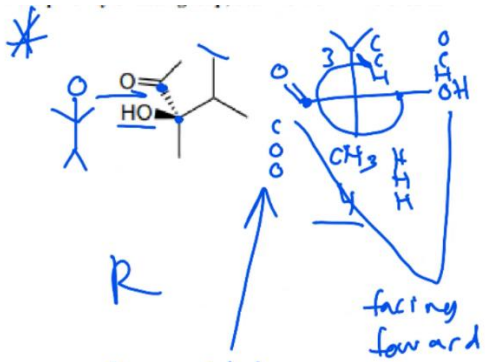
C_xH_{2x+2}

3 DU / 3 ° unsat

2D) (6 pts) Identify the configuration (e.g., *R*, *S*) for each of the following compounds. **Show your work to receive credit - i.e., show the priority of each group, etc. No work = no credit.**

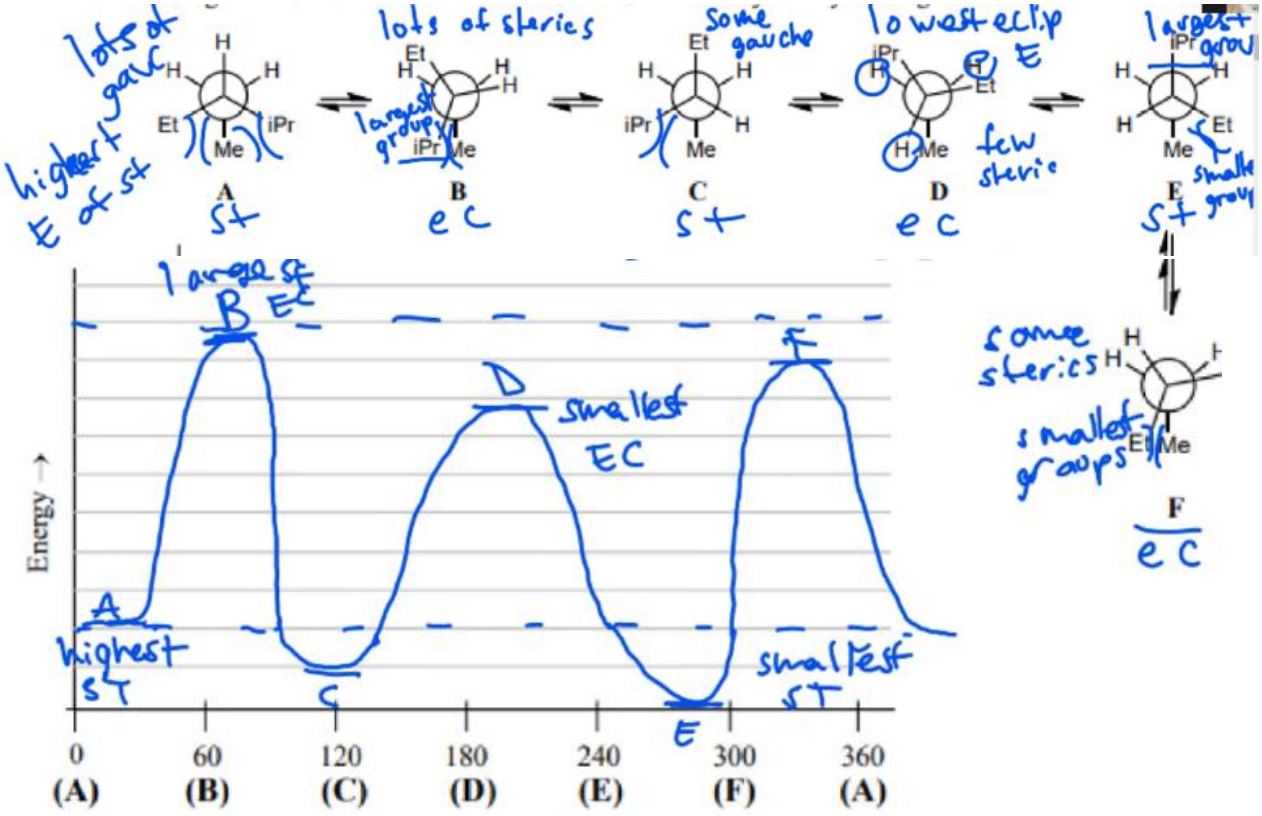


H on wedge, must reverse so lowest group on dash

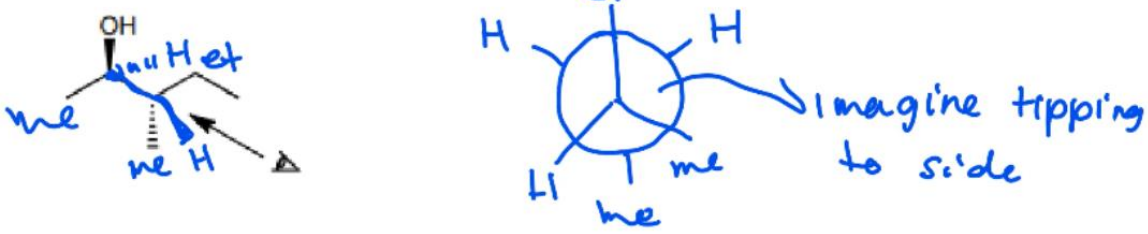


C would be approached 1st, makes COO less important

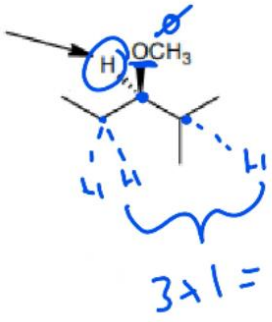
3A) (10 pts) Given the Newman projections below, sketch an energy diagram showing the relative energies of the conformers. Start with **A** at 0° and clearly label your diagram.



3B) (5 pts) Draw a Newman projection of the following compound, as viewed from the angle indicated.



3C) (4 pts) For the highlighted proton(s), consider its expected signal in a ^{1}H NMR spectrum. Describe the expected integration (e.g, 1H/2H/3H/etc.), multiplicity/splitting pattern (e.g. s/d/t/e and approximate chemical shift (δ value, you may refer to table on page 6).



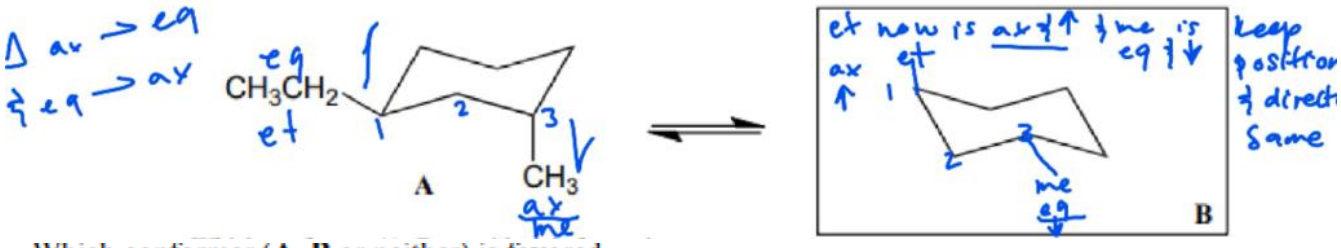
integration: 1 H

splitting pattern: quartet looking at neighbors

approximate δ = 3.8 ppm

R O - CH3

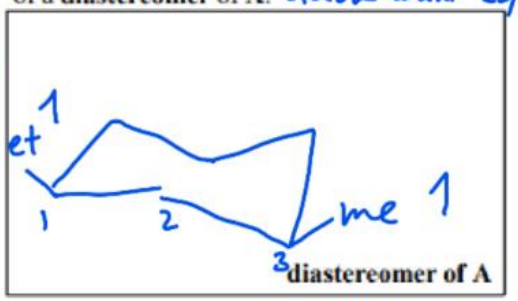
4A) (12 pts) Perform a ring flip on **A** to draw the other chair conformation (**B**), and answer questions.



Which conformer (**A**, **B** or neither) is favored at equilibrium? Explain briefly.

Is **A** the cis or trans isomer?

Draw the most stable chair conformation of a **diastereomer** of A.

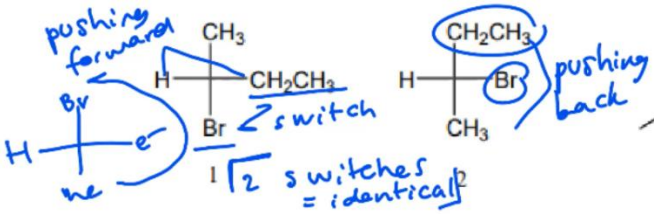


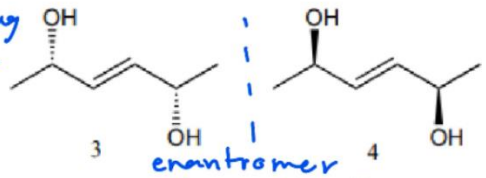
4B) (12 pts)
What is the relationship of the following pairs of compounds?

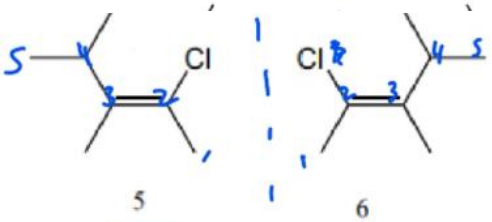
1 and 2 D 3 and 4 _____

5 and 6 D 7 and 8 _____

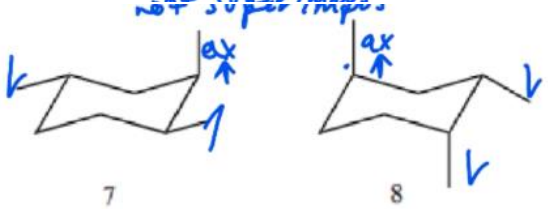
A) constitutional (structural) isomers
B) enantiomers
C) diastereomers
D) the same compound
E) unrelated

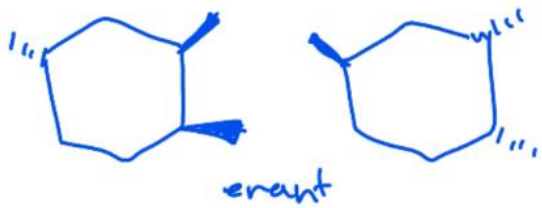






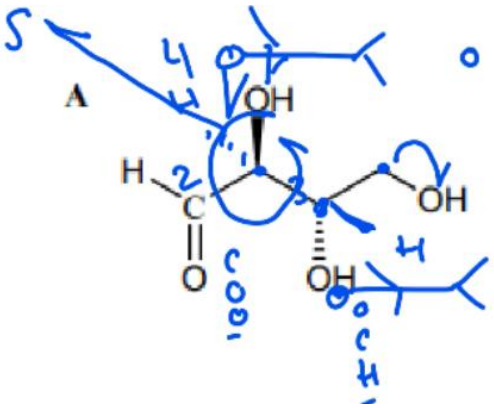
Superimpos same molec

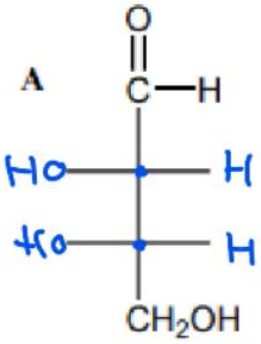




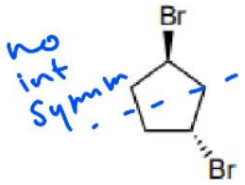
enant

5A) (4 pts) Complete the Fischer projection for compound **A**.



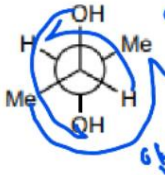


5B) (6 pts) Determine whether each of the following compounds is **chiral** (yes/no) and whether or not it **has an enantiomer** (yes/no).



chiral? yes

has an enantiomer? yes



chiral? no

has an enantiomer? no

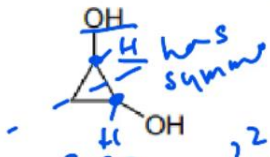
5C) (4 pts) Describe the optical activity for each of the samples given below, using choices a-d.

racemic mixture of tartaric acid: C

(*R*)-(−)-ibuprofen that is 96 % e.e.: B

a) dextrorotatory
b) levorotatory
c) optically inactive
d) can't tell (need more info.)

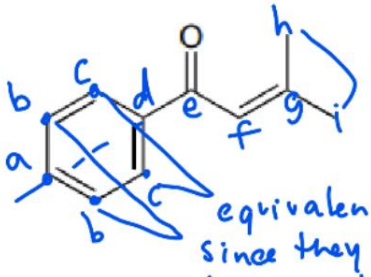
5D) (4 pts) On the following compound, mark all the chiral centers with an asterisk (*) and indicate how many stereoisomers it has (you do not need to draw them).



total number of stereoisomers: 3

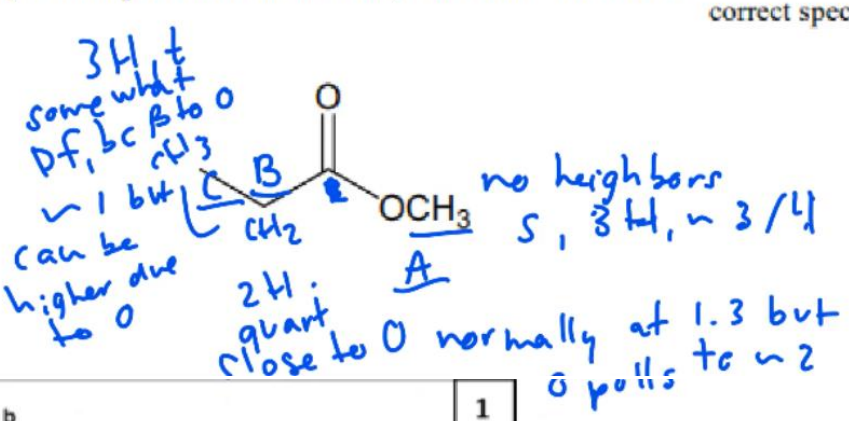
5E) (6 pts) How many signals are expected in the ^{13}C NMR spectrum of the given compound? Label each carbon atom a/b/c/etc. to indicate any that are equivalent.

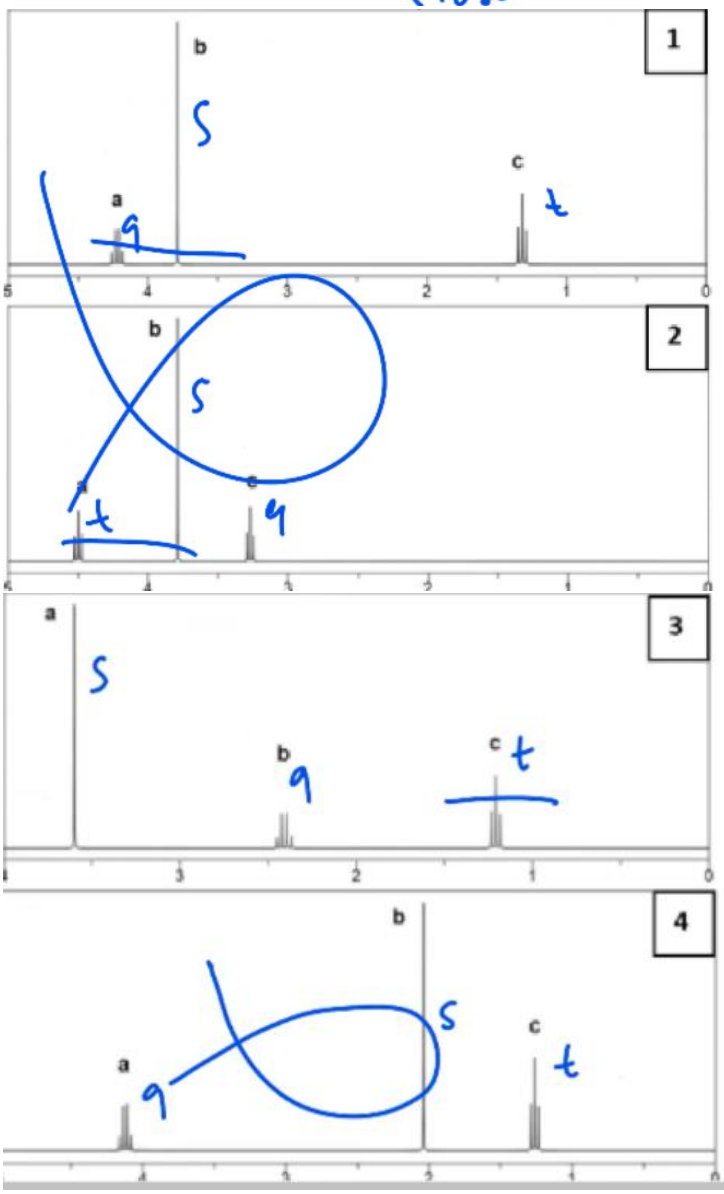
Total number: 9



6) (8 pts) Identify the ^{1}H NMR spectrum (1/2/3/4) that corresponds to the given structure, and **label the protons on the structure a/b/c** to match the signals in the spectrum. Show your work to justify your choice (i.e., why is that spectrum is the best fit?). **No work = no credit.**

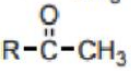
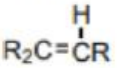
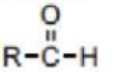
correct spectrum: C





^{1}H NMR

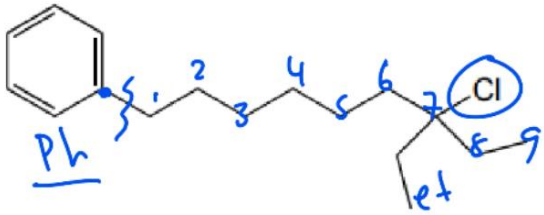
Protons on Carbon

Type of C-H	δ (ppm)
$R-CH_3$	0.9
$R-CH_2-R$	1.3
R_3C-H	1.5-2
	1.8
	2-2.3
$Ar-CH_3$	2.3
$RC\equiv C-H$	2.5
R_2N-CH_3	2-3
$R-CH_2-X$	3-3.5
$RO-CH_3$	3.8
$R-CH_2-F$	4.5
	5-5.3
$Ar-H$	7.3
	9.7

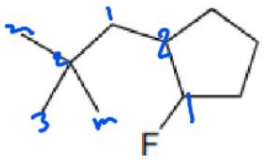
Protons on Oxygen

Type of H	δ (ppm)
ROH	0.5-5
ArOH	4-7
	10-13

I. A) Nomenclature (12 pts) Name the following compounds according to the IUPAC rules. Be sure to indicate stereochemistry, when appropriate. **You must show your work for full credit.**



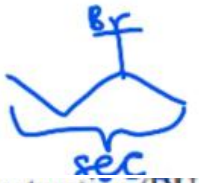
7-chloro-7-ethyl-1-phenylheptane



2 + 3 = 5

1-Fluoro-2-(2,2-dimethylpropyl)cyclopentane

Draw *sec*-butyl bromide



B) (8 pts) Determine the degrees of unsaturation (DU or HDI) for the following compound. **Show your work for full credit.**

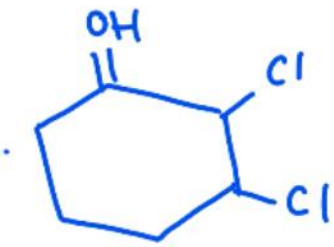
$C_6H_8OCl_2$ DU: 2DU

$C_6H_{10} \longrightarrow C_6H_{14}$ = 4 H diff → 2 DU

C_xH_{2x+2}

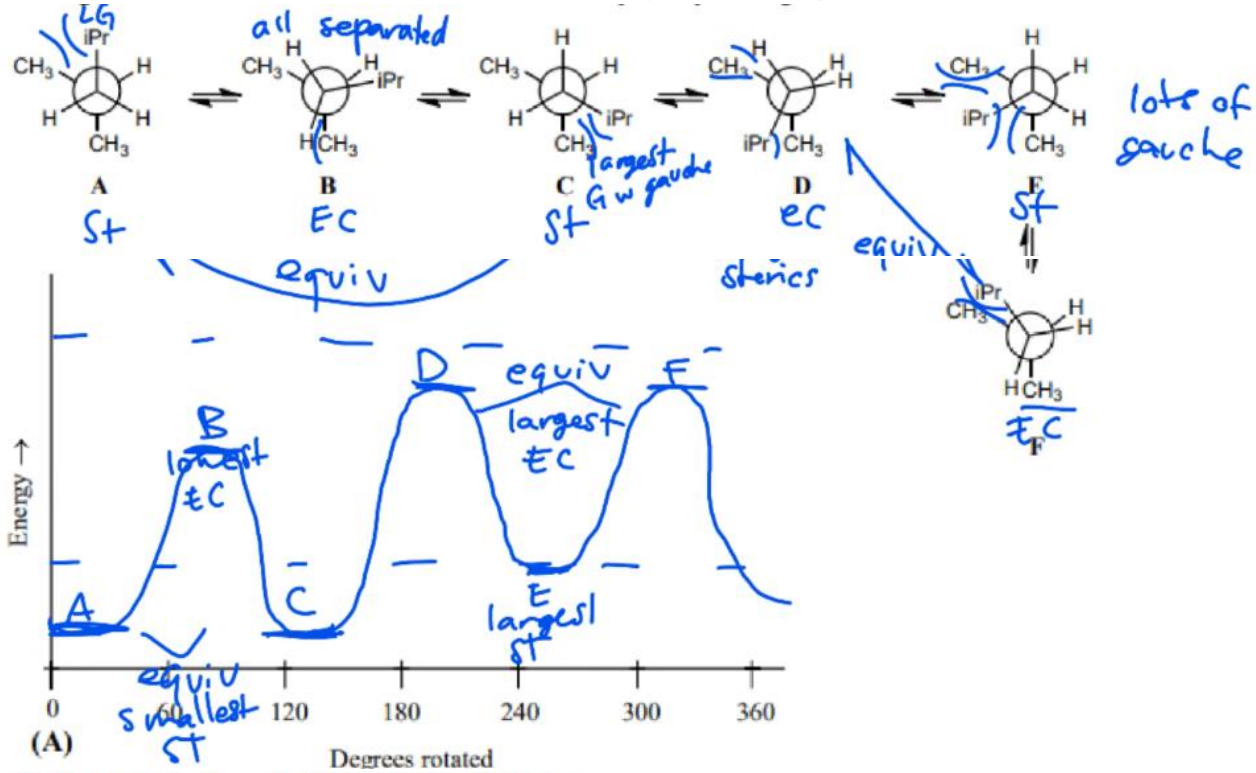
Draw two **constitutional isomers** of $C_6H_8OCl_2$ (there are many possible answers).

$C_6H_{10} \longrightarrow C_6H_{14}$ 2° DU



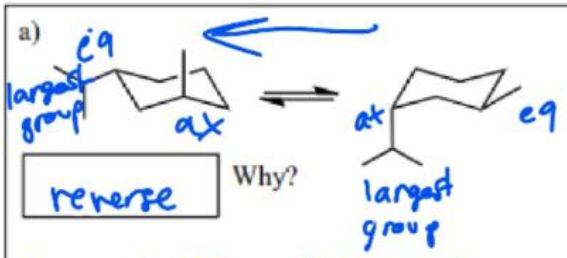
II. (18 pts)

A) (10 pts) Given the Newman projections below, sketch an energy diagram showing the relative energies of the conformers. Start with **A** at 0° and clearly label your diagram.



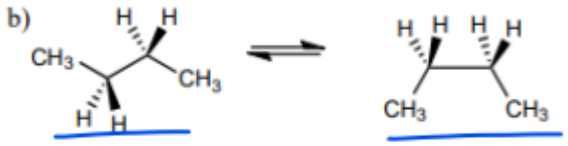
B) (8 pts) In the box provided for each equilibrium, indicate which direction (forward, reverse or neither) is favored and briefly explain why. **No explain = no credit.**

a)



reverse Why? lowest E will be when largest group on eq & more stable.

b)



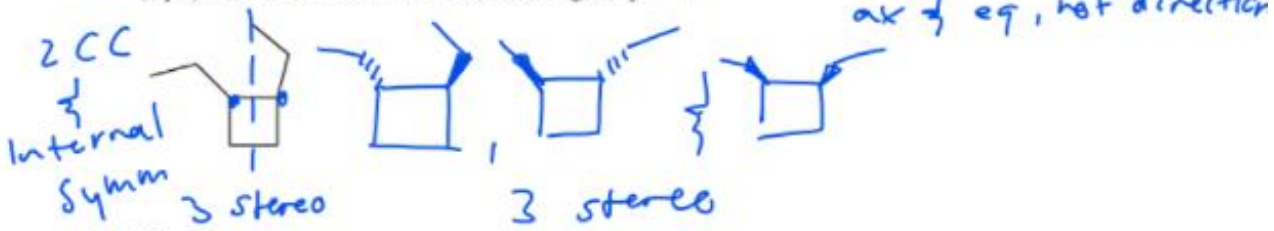
neither Why? same molec no direction

III. (22 points)

(5 pts) Shown below is a chair conformation of a substituted cyclohexane (**A**). Using the chair given below, draw the other chair conformation (**B**). (No comparison or explanation is required.)

only switching ax & eq, not direction

(5 pts) Draw all stereoisomers of the following compound:



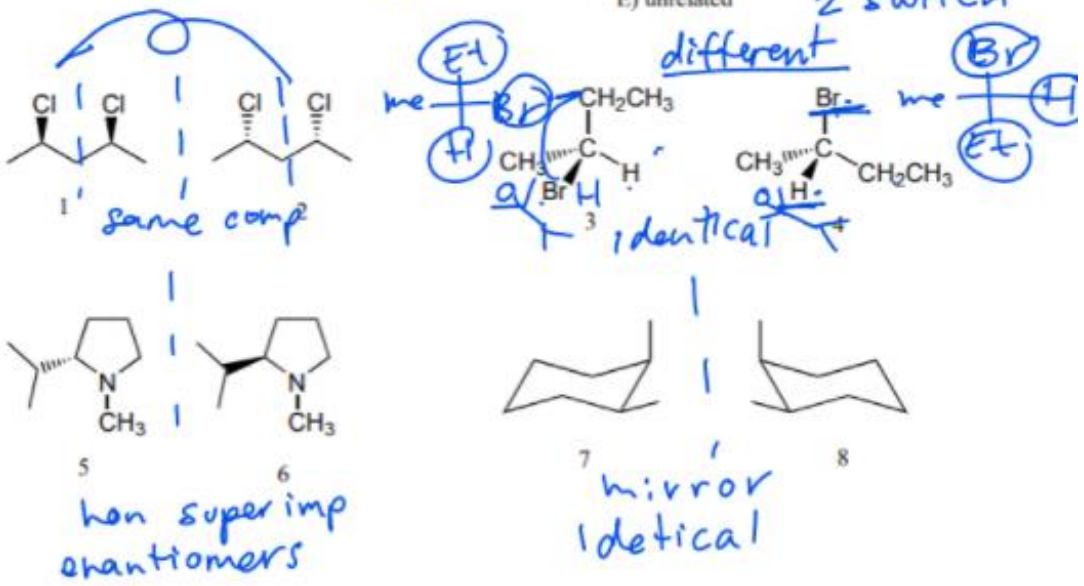
(12 pts)

What is the relationship of the following pairs of compounds?

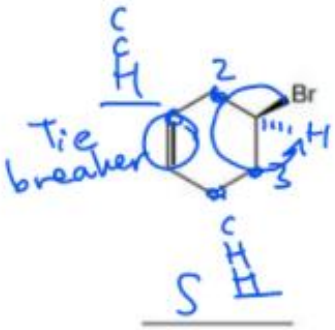
1 and 2 D 3 and 4 D

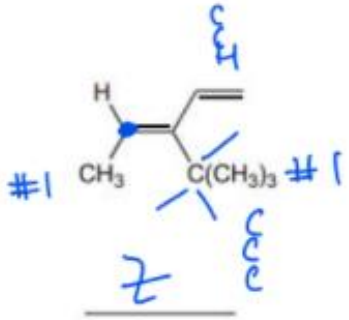
5 and 6 B 7 and 8 D

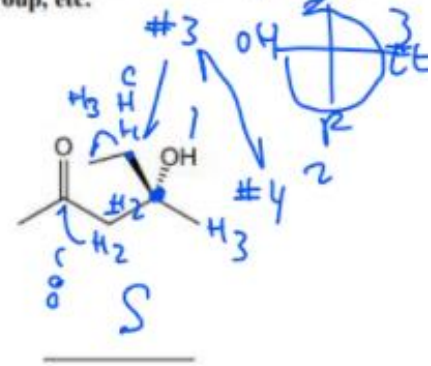
A) constitutional (structural) isomers
B) enantiomers
C) diastereomers
D) the same compound
E) unrelated



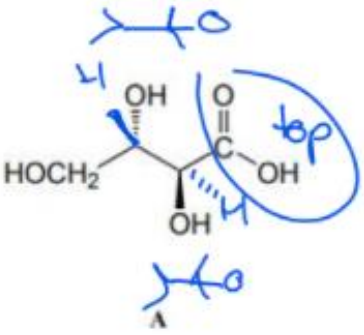
IV. (9 pts) Identify the configuration (e.g., *R, S, E, Z*) for each of the following compounds. **Show your work to receive credit - i.e., show the priority of each group, etc.**

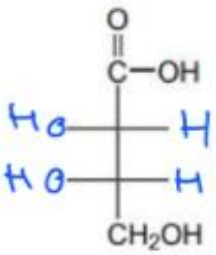




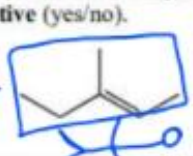


(4 pts) Complete the Fischer projection for compound **A**.





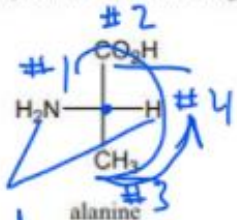
(3 pts) Determine whether the following compound is **chiral** (yes/no) and whether or not it is **optically active** (yes/no).



chiral? no

optically active? no

(8 pts) Answer the following questions, using the given structure of naturally occurring alanine.



What is the configuration of alanine (e.g., *R, S*)? S

Is alanine chiral? yes 4 unique groups

Does alanine have an enantiomer? yes

What do you expect for the optical rotation [α] for alanine? d
a) dextrorotatory; b) levorotatory; c) neither; d) can't tell

^{13}C NMR: Carbons

Type of carbon	δ (ppm)	Type of carbon	δ (ppm)
R–CH_3	10-30		
C–O	40-80	R–C(=O)–OR	165-185
RC≡CR	65-90	R–C(=O)–NH_2	
$R_2C{=}CR_2$	100-150		
	110-170	R–C(=O)–R/H	185-220

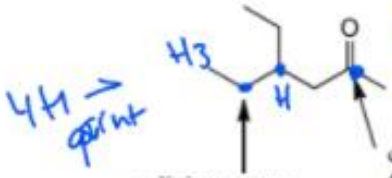
^{1}H NMR
Protons on Carbon

Type of C-H	δ (ppm)
R–CH_3	0.9
R–CH_2–R	1.3
R_3C–H	1.5-2
	1.8
R–C(=O)–CH_3	2-2.3
Ar–CH_3	2.3
RC≡C–H	2.5
R_2N–CH_3	2-3
R–CH_2–X	3-3.5
RO–CH_3	3.8
R–CH_2–F	4.5
$R_2C{=}CR$	5-5.3
Ar–H	7.3
R–C(=O)–H	9.7

Protons on Oxygen

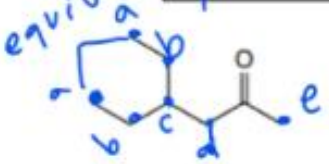
Type of H	δ (ppm)
ROH	0.5-5
ArOH	4-7
R–C(=O)–OH	10-13

(8 pts) Refer to the given compound to answer the following questions.



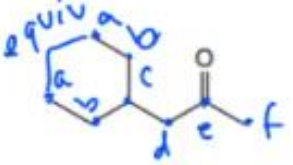
splitting pattern for this proton: quintet

chemical shift for this carbon: 185-220 CNMR



Number of signals in ^{1}H NMR: (label protons a/b/c/etc.)

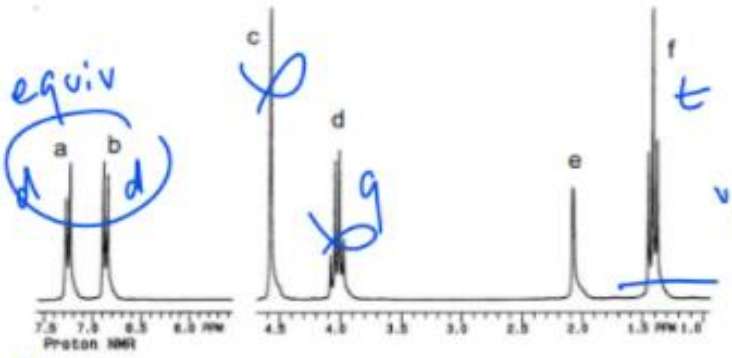
5

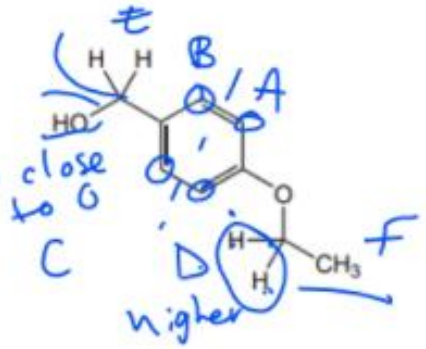


Number of signals in ^{13}C NMR: (label carbon atoms 1/2/3/etc.)

6

(8 pts) Match the labeled peaks in the ^{1}H NMR with the protons on the given structure.
(Label the protons on the structure a/b/c/etc.)





further DF = closer to O