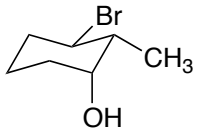
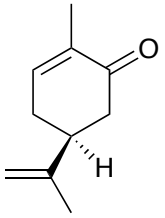
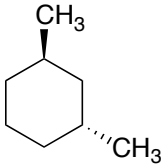
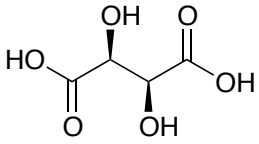
Homework Four

Organic Chemistry I (223) • Prof. Chad Landrie
Spring 2013

Completion (6 pts)		**Name**	
Random Sample(s) (4 pts)		**BID**	
Total (10 pts)		**Section-CRN**	

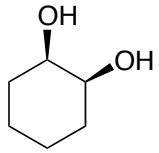
Additional Recommended Problems from McMurray (8th Ed.)	

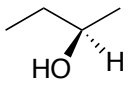
1. Draw the enantiomer for each of the following molecules.

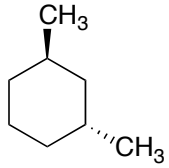
			
			

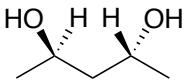
2. Label each chirality center in your drawn molecules above and the original molecules above as *R* or *S*.

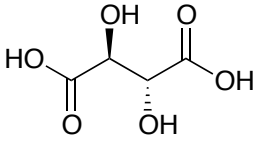
3. Circle the molecules below that are meso.

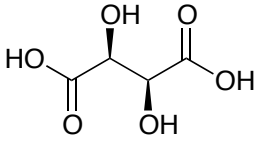


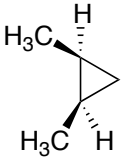


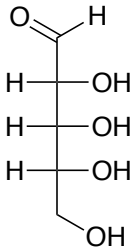


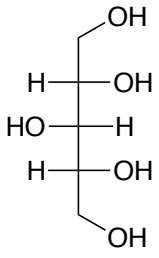


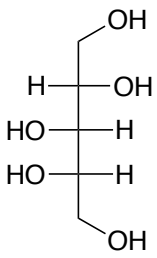












4. Define meso. Are meso compounds optically active? Why or why not?

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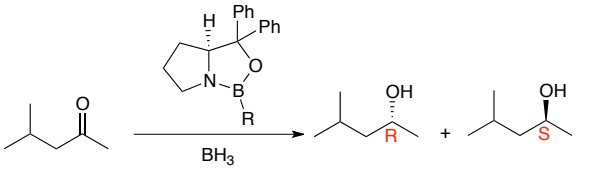
5. Ketones can be reduced to alcohols enantioselectively (one enantiomer is preferred) by using a chiral catalyst such as the one shown below. If the specific optical rotation for the product mixture formed by this reduction was –12.0°, what was the enantiomeric excess for this reaction? In the boxes, list the percent of each compound in the product mixture. Show all work.



$[\alpha]_S$ = +18.5°

enantiomeric excess (ee)?

6. Draw each of the following showing the correct stereochemistry at each chirality center.

a. (*R*)-2-methylpentane

b. (2*R*, 3*S*)-2,3-dibromobutane

c. meso form of 3,5-heptanediol (diol = 2 OH groups)

d. most stable chair of (1*R*, 2*R*)-1-isopropyl-2-methylcyclohexane

7. What will be the observed specific optical rotation when a 1.2 M solution of (*R*)-2-butanol is mixed with an equal volume of a 0.560 M solution of racemic 2-butanol. The resulting solution is analyzed in a sample container that is 10.0 cm long. The specific optical rotation of (R)-2-butanol is –13.9° mL g^{-1} dm^{-1}? Show all work.

8. Sucrose has a specific optical rotation of 66.5°. If a solution of pure sucrose is found to have an optical rotation of +23°, what is the concentration of the solution?

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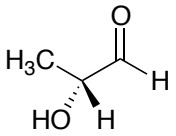
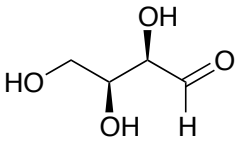
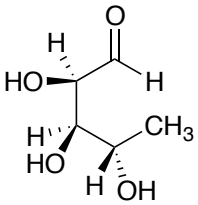
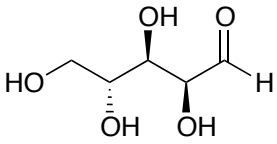
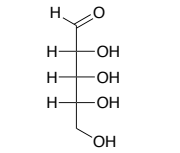
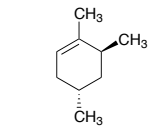
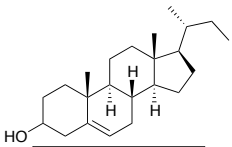
9. Draw Fisher projections for each of the following molecules that places the aldehyde functional group at the top.

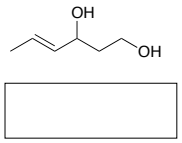
			
			

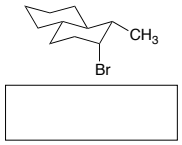
10. Determine how many possible stereoisomers there are for each compound.

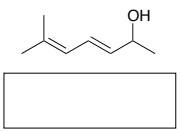






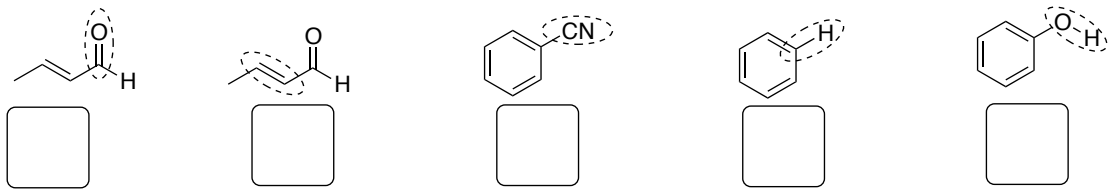






11. Describe the difference between enantiomers and diastereomers in terms of configuration, properties as well as optical rotation.

12. Rank each circled bond in order of increasing wavenumber ("frequency") for the stretching motion in infrared spectroscopy (1 = lowest wavenumber; 5 = highest wavenumber).



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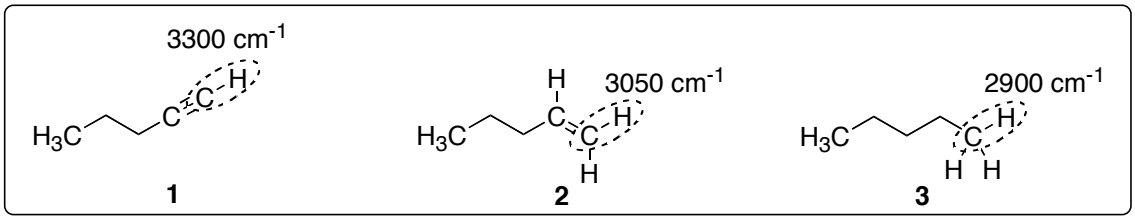
13. Briefly state the variation in IR stretching frequency for the C-H bonds in the molecules below. Include a discussion of hybridization, the orbital overlaps that makeup the C–H σ-bond, bond strength and Hooke's law. You may also draw diagrams (e.g., molecular orbitals) if they will aid in your discussion.



14. Conjugated (adjacent π-bonds) carbonyl compounds have a lower stretching frequency than non-conjugated carbonyl bonds. First, draw an example of a conjugated ketone and a non-conjugated ketone. Second, state what two factors affect the IR stretching frequency of a covalent bond. Third, explain why the conjugated ketone has a lower stretching frequency. You will need to draw additional diagrams to illustrate your answer.

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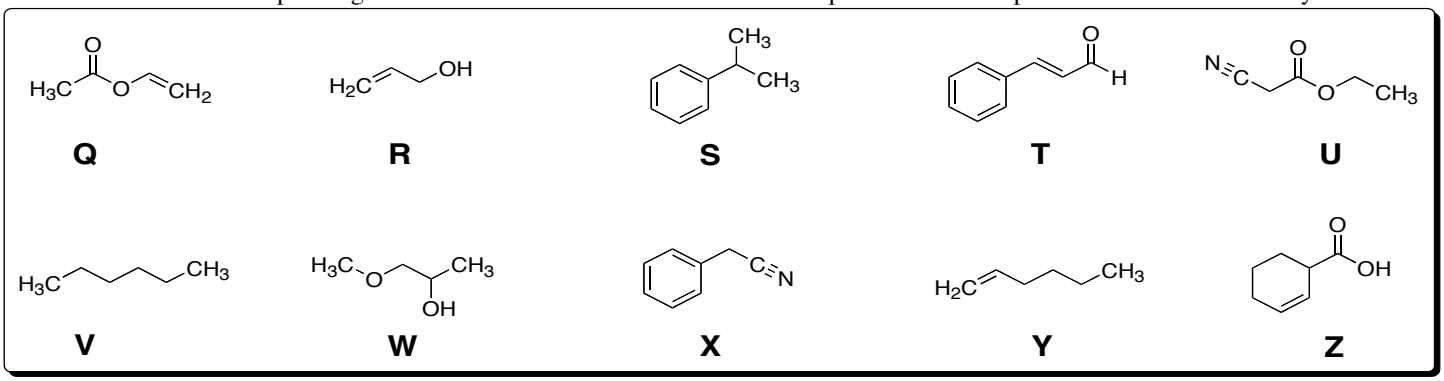
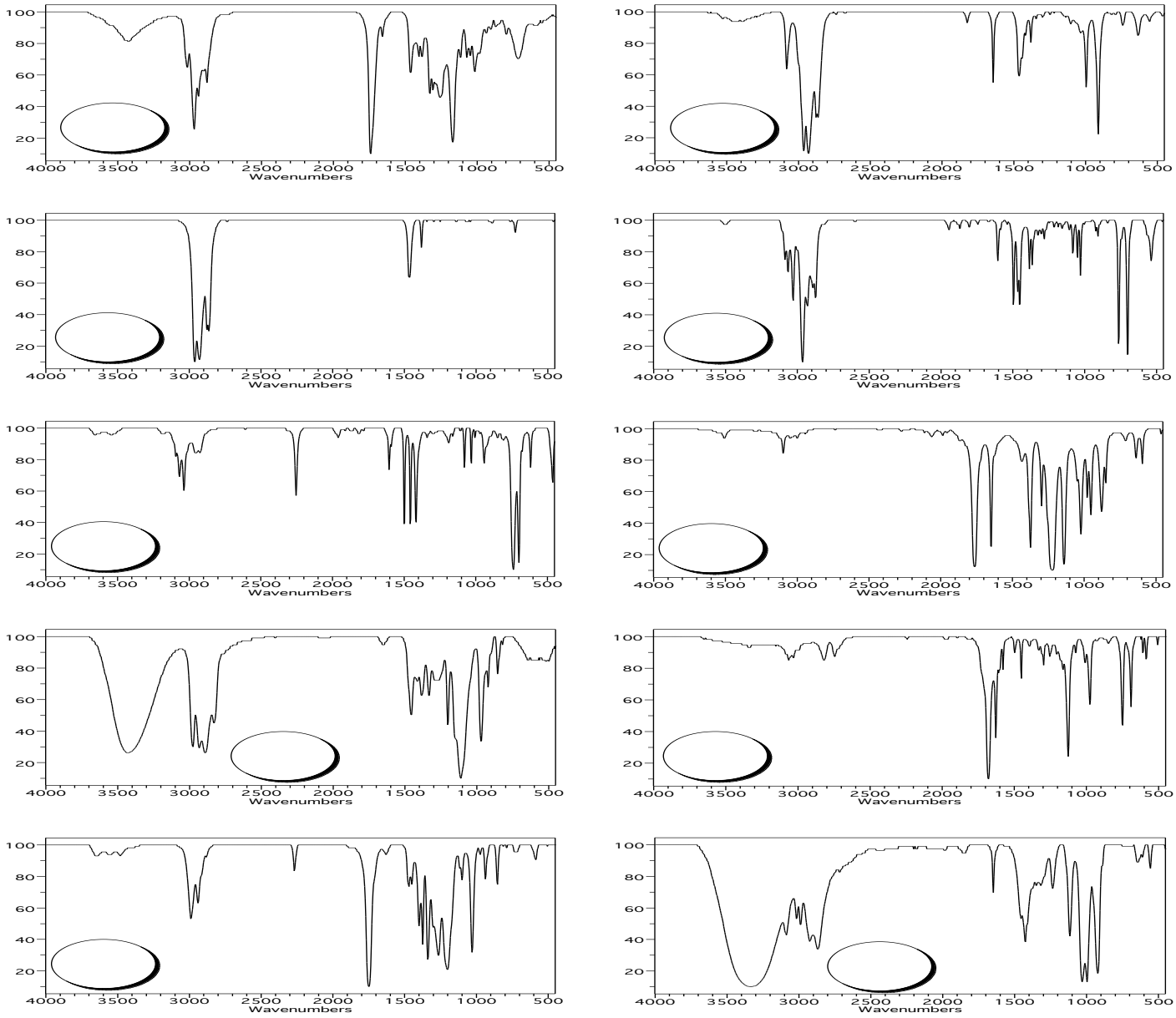
15. Write the letter corresponding to each molecule in the circle within its respective infrared spectrum. Each letter is only used once.





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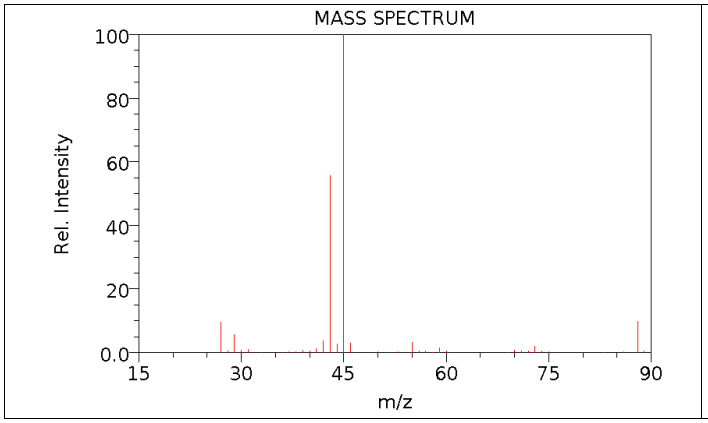
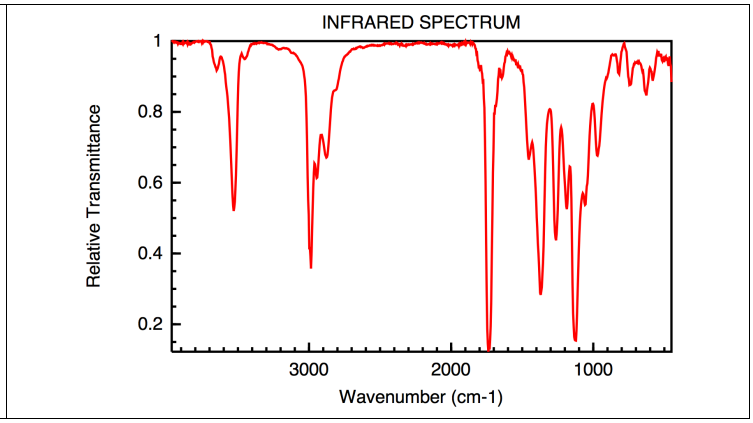
16. The CSI lab found traces of an unknown substance at the scene of a crime. It was found to be soluble in CH_2Cl_2, but insoluble in either aqueous acid or aqueous base. Elemental analysis of the substance was found to contain: 54.53% C, 9.15% H, and 36.32% O by mass. Infrared and mass spectra were also acquired. Unfortunately, the compound did not match any substances in their library so they had to call in real chemists (you!) to deduce the structure.





a. First, determine the molecular formula from the elemental analysis and MS data. Show all work.

b. Second, determine the index of hydrogen deficiency (the number of double bonds and/or rings) from the molecular formula.

c. Third, list the functional groups indicated by the IR spectrum and then draw your proposed structure below.

d. Based on your structure above, draw two cation (or radical cation) fragments that could account for the m/z signals at 43 and 45.