

Name:

CHEMISTRY 249S
Examination 1
February 8th 2007

Answer all questions in the spaces provided on the examination sheets,
indicating clearly what is to be graded.

**PRINT YOUR NAME AND STUDENT NUMBER
CLEARLY ON THE FIRST PAGE OF THE EXAM BOOKLET**

NAME:

STUDENT NUMBER:

NMR Spectroscopic Correlation Tables are provided on Pages 9-10
of this booklet.

Allowed Aids: Molecular Models

Calculators and other electronic devices are not permitted in this examination

Credit will be given for partial answers

WAIT UNTIL YOU ARE TOLD TO BEGIN

Marking Scheme

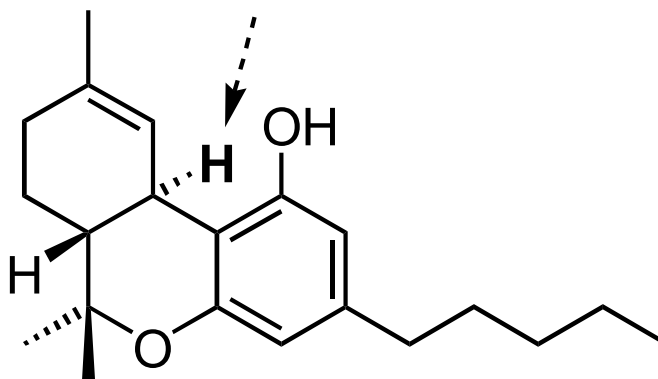
Good Luck!



Question 1	20	
Question 2	25	
Question 3	25	
Question 4	60	
Total	130	

Name:

1. (20 Points) Shown below is the chemical structure of Δ^9 -tetrahydrocannabinol (THC), the major psychoactive compound isolated from the plant *Cannabis sativa*. Answer the following questions about the structure of this compound.

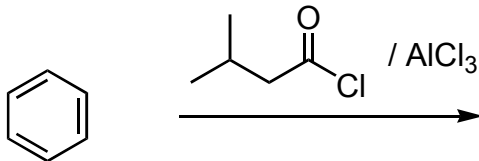


- (a) How many chiral centres (stereogenic carbon atoms) are there in this molecule?
- (b) What is the stereochemical assignment of the alkene?
- (c) What is the index of hydrogen deficiency (degree of unsaturation) of the molecule?
- (d) How many distinct methyl group signals would you expect to see in the DEPT NMR?
- (e) How many DEPT signals (peaks) do you expect to see in the ^{13}C NMR downfield of 100.0 ppm?
- (f) What splitting pattern (multiplicity) would the highlighted proton (i.e., the one indicated by the dashed arrow) show in the ^1H NMR? (You may assume that only 2- and 3-bond couplings occur)
- (g) On addition of D_2O to an NMR sample of Δ^9 -THC, one or more of the peaks disappear from its ^1H NMR spectra. On the structure above, indicate which proton(s) are affected.
- (h) What is the most upfield signal that you would expect to see in the ^1H NMR? Indicate this on the structure above by drawing a circle around the relevant hydrogen atom(s).

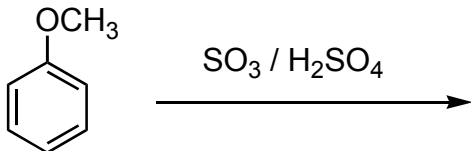
Name:

2. (25 Points) What are the major products of the following reactions? You should clearly indicate the selectivity of the reactions. It is NOT required to draw mechanisms for your transformations.

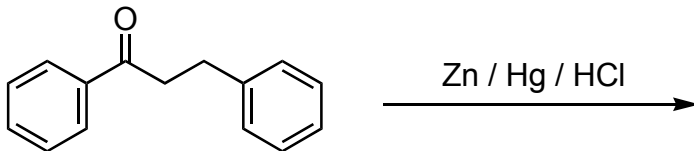
(a)



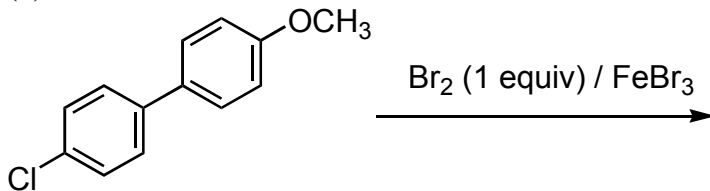
(b)



(c)

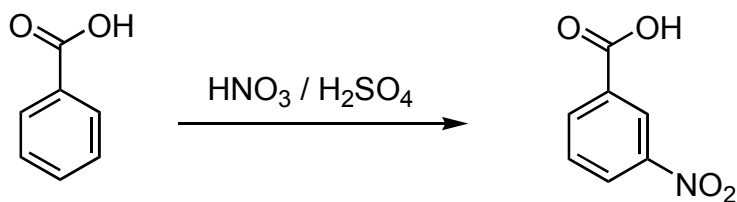


(d)



Name:

3. (25 Points) Answer the following questions about the reaction shown below.



- (a) Draw a full mechanism for this transformation. Your answer should include curved arrows to show electron movement.

- (b) Explain why the meta isomer is the predominant product.

- (c) Is the product more or less reactive toward further electrophilic aromatic substitution than the reactant (i.e., benzoic acid)? Briefly explain your reasoning.

Name:

4. **(60 Points)** The spectral data for three unknown compounds, **A**, **B** and **C**, are given on the next 3 pages. Deduce the structures for the unknown compounds. Please note, even if you cannot deduce the final structures, marks will be given for fragments of those structures or your deductive reasoning. Also, only 2 and 3-bond couplings are given in the ^1H NMR spectra.

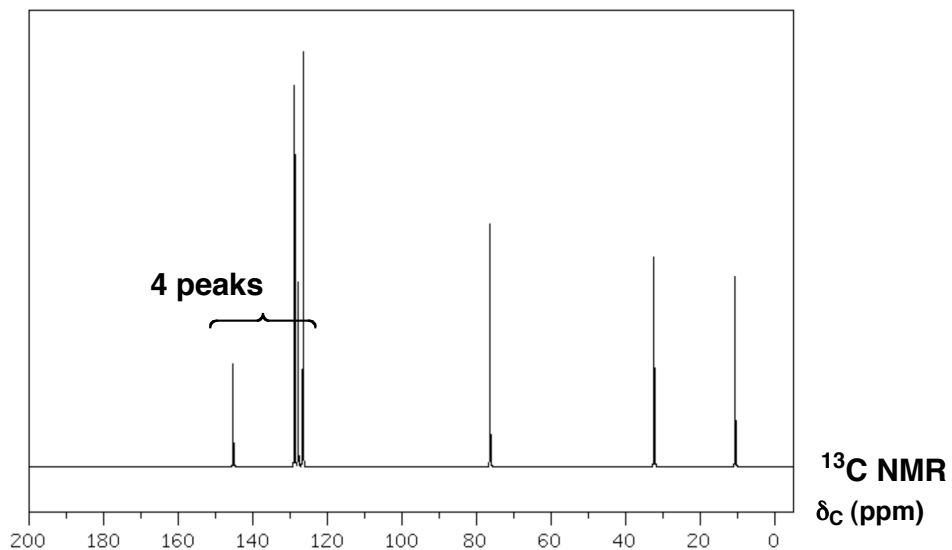
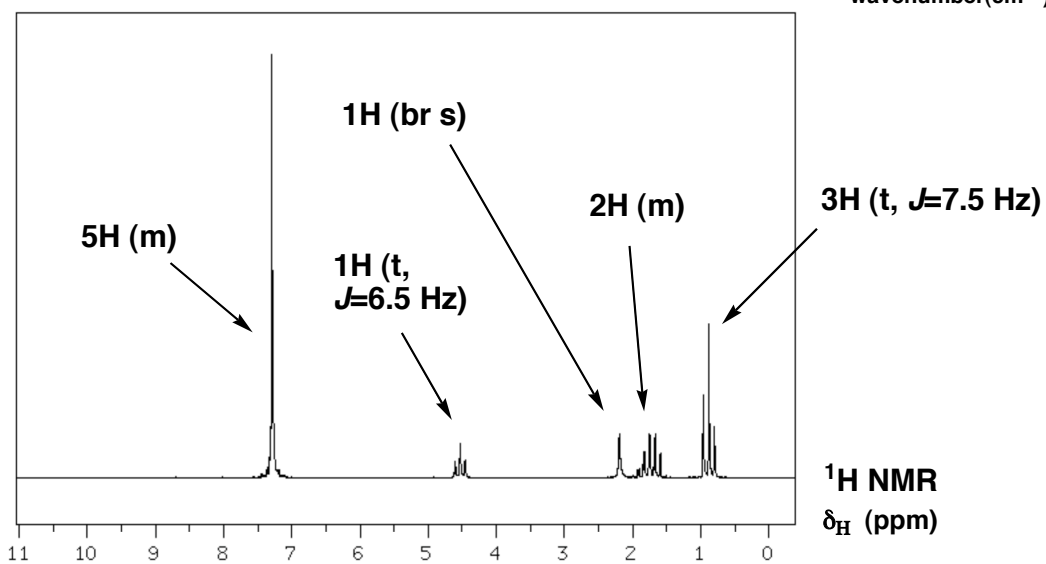
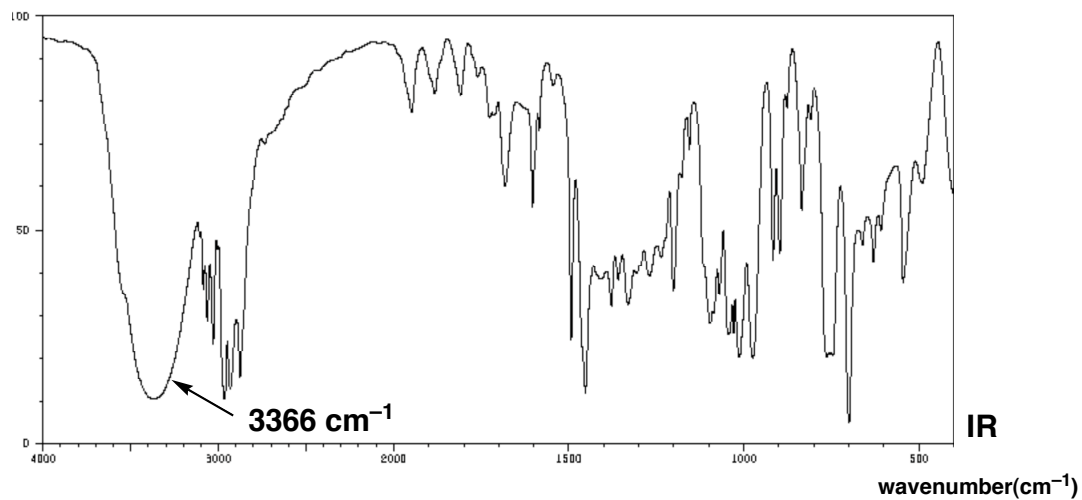
COMPOUND A:

COMPOUND B:

COMPOUND C:

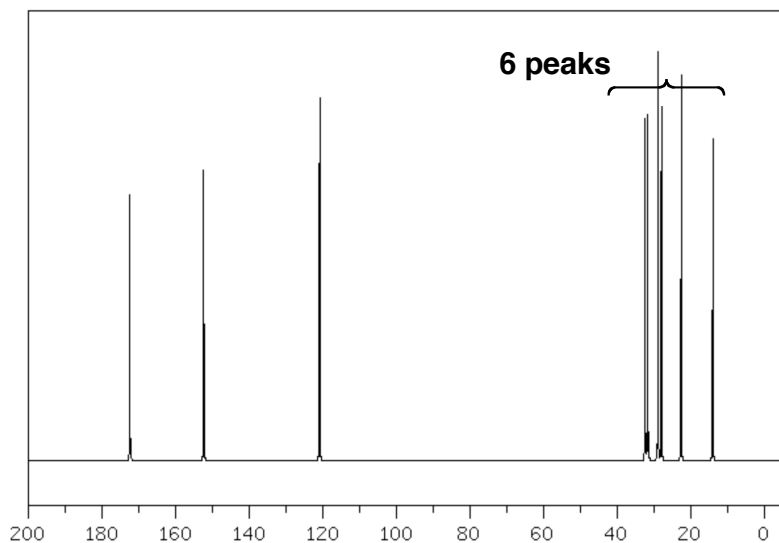
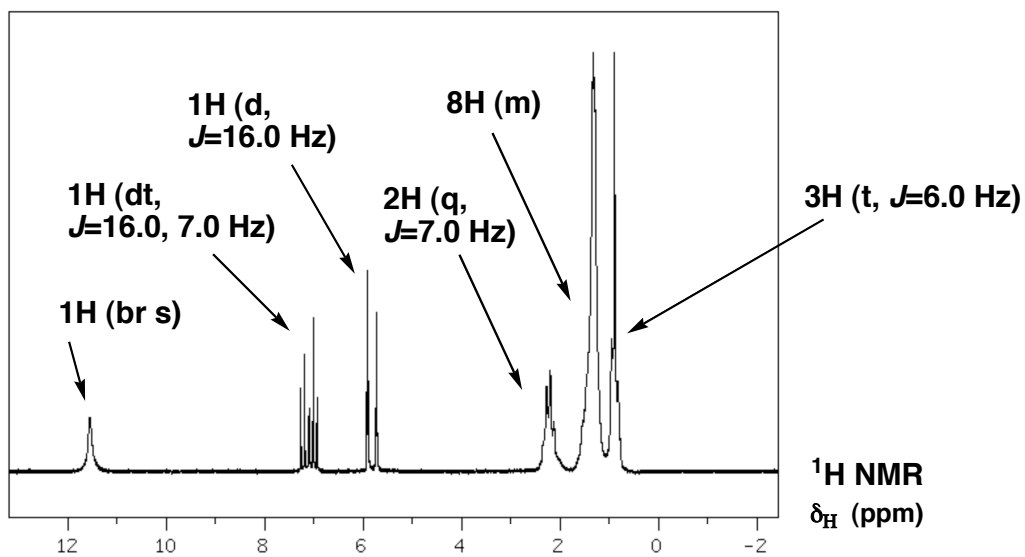
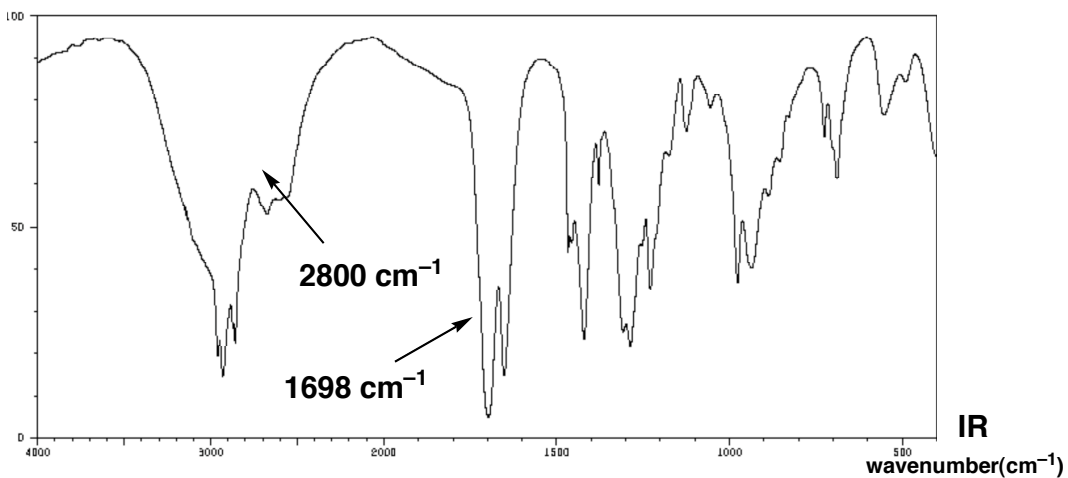
Name:

COMPOUND A:
Molecular Formula = $C_9H_{12}O$



Name:

COMPOUND B:
Molecular Formula = C₉H₁₆O₂

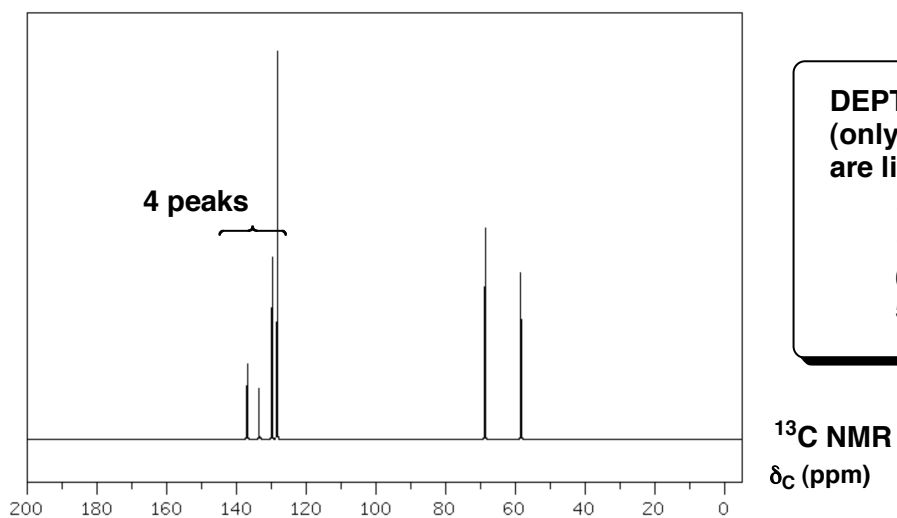
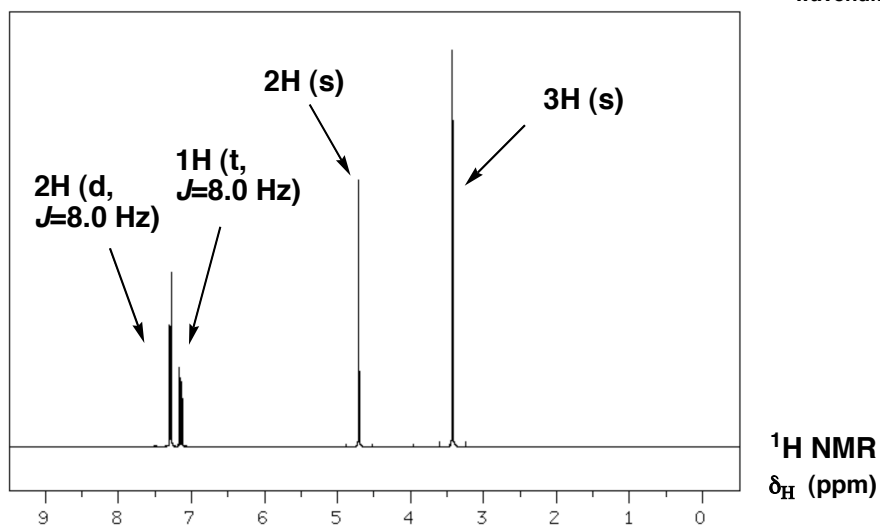
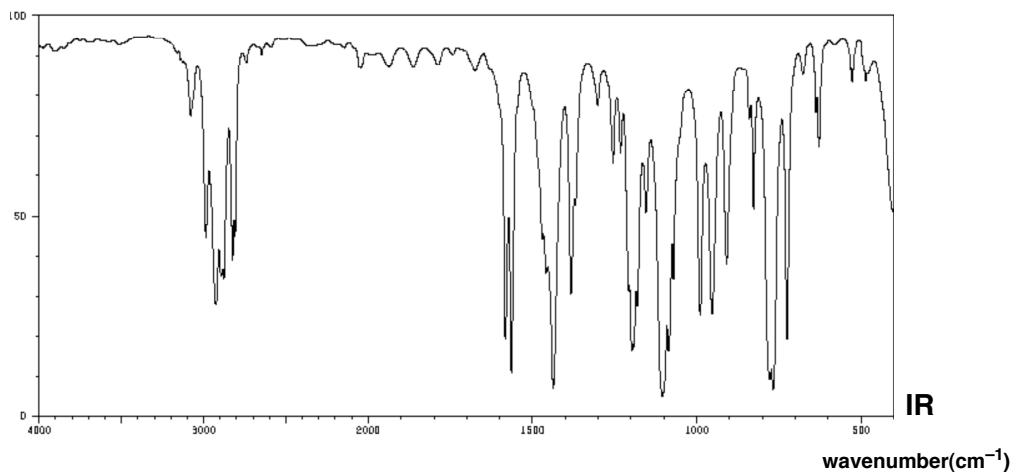


DEPT NMR δ_C (ppm)
(only protonated C's are listed)

152.4	CH
120.9	CH
32.4	CH ₂
31.7	CH ₂
28.9	CH ₂
28.0	CH ₂
22.6	CH ₂
14.0	CH ₃

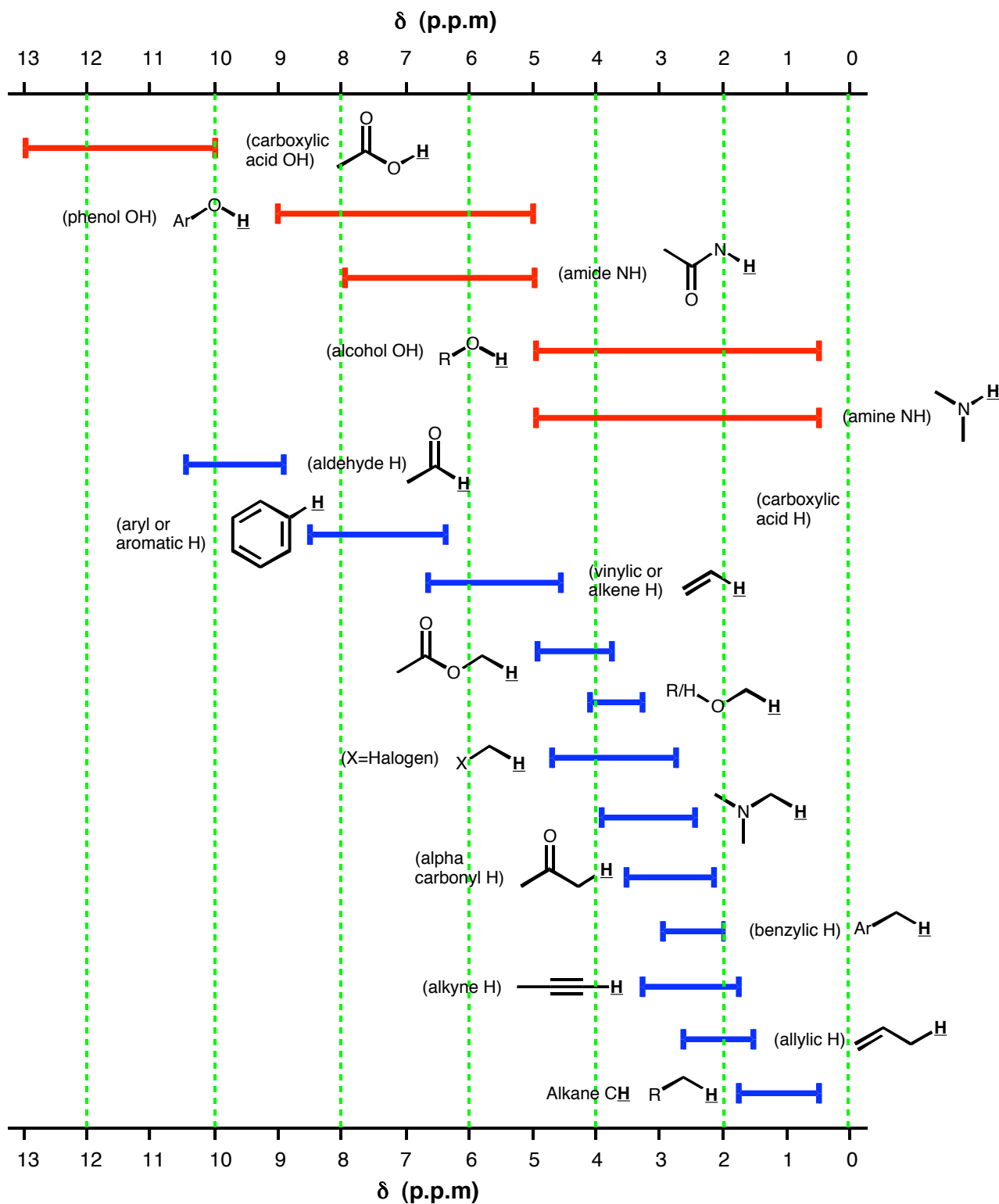
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COMPOUND C:
Molecular Formula = C₈H₈Cl₂O



Name:

Proton Chemical Shifts

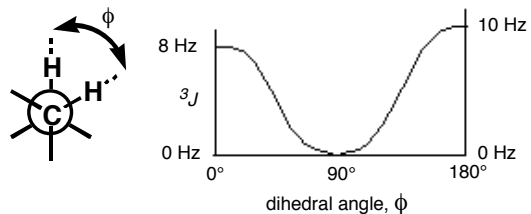
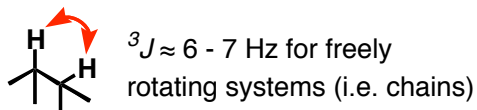


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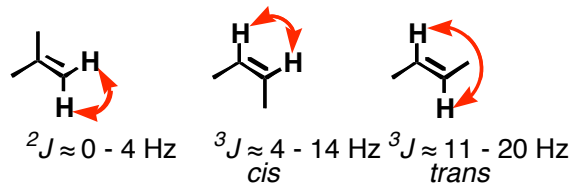
Abbreviations for proton multiplicities: s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet.
Higher multiplicities are given in full i.e. quintet, sextet, septet, etc.

Coupling Constants (J values)

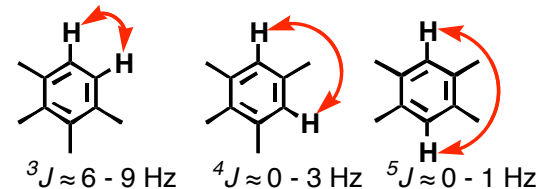
Aliphatic Protons:



Alkene Protons:



Aromatic Protons:



^{13}C Chemical Shifts

