Organic 211
Assignment # 18
Fall 2020

Name:_____

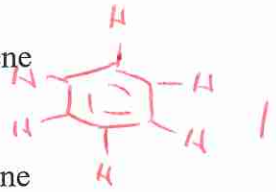
Proton NMR has four questions that allow you to work any NMR problem.

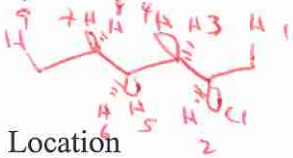
Enantiotopic, Diasterotopic, and homotopic protons

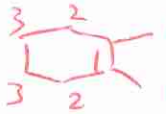
1) For the following molecules, indicate how many different sets of protons you would expect to find in the proton NMR. Assume this is in an ACHIRAL solvent (e.g. CH2 protons won't be different if no chiral center is present)

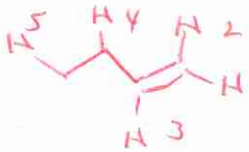
a) Ethane — 1

b) Neopentane + 1

c) Benzene  1

d) R-2-chlorohexane  (9)

e) 1,2-dimethylcyclohex-1-ene  (3)

f) 1-butene  (5)

Location

2) Another question is LOCATION. Where do the protons show up? Using a chart, indicate where the protons show up.

a) Ethane

1.25 δ

b) Neopentane

0.902 δ

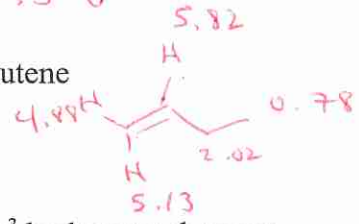
c) Benzene

7.3 δ

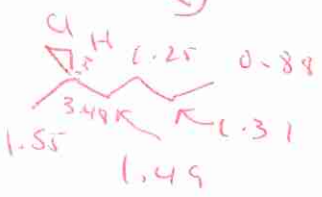
d) R-2-chlorohexane 

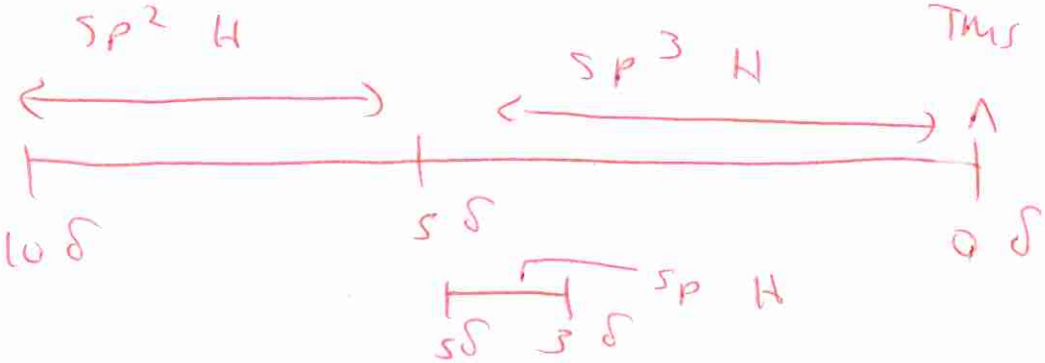
e) 1,2-dimethylcyclohex-1-ene

1.79 1.76 1.79

f) 1- butene 

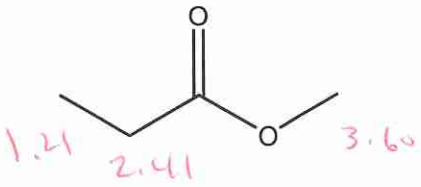
3) Draw the proton NMR spectrum from 10 δ to 0 δ. a) Indicate where sp^3 hydrogens show up relative to TMS. b) Indicate where sp^2 hydrogens usually show up relative to TMS. c) Indicate where sp hydrogens up relative to TMS.



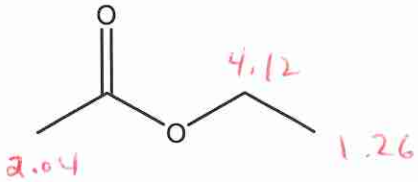


4) Indicate the location of the protons for the following molecules. Put a number by the protons.

a) Methyl propanate



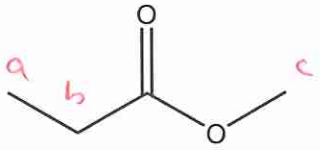
b) Ethyl acetate

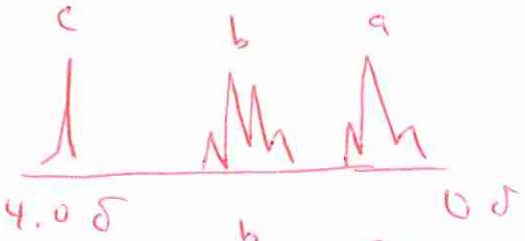


Splitting Patterns

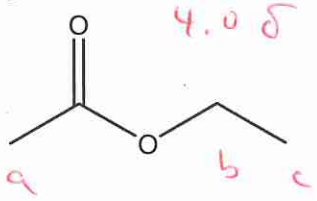
5) Assuming the coupling constant is the same (e. g. Jab is the same as Jbc, which is not usually the case), use the N + 1 rule and assign how each proton would show up in the proton NMR.

a) Methyl propanate



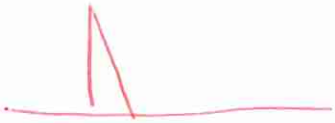


b) Ethyl acetate



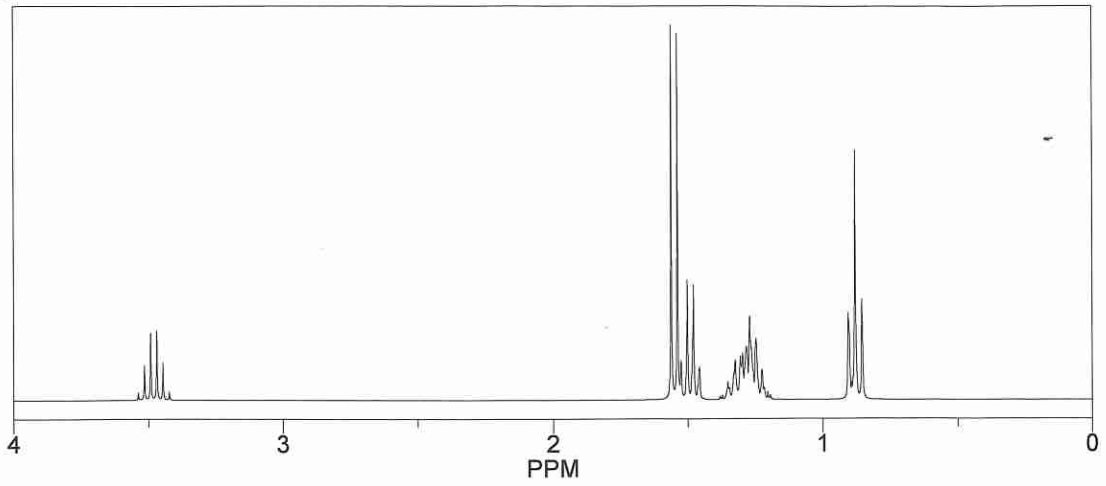
c) Ethane

d) Neopentane

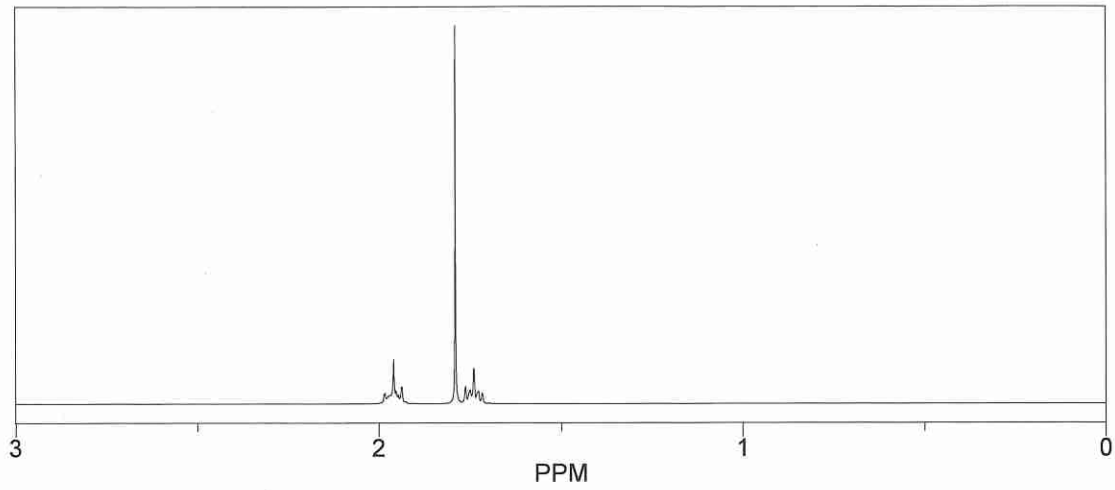


e) Benzene

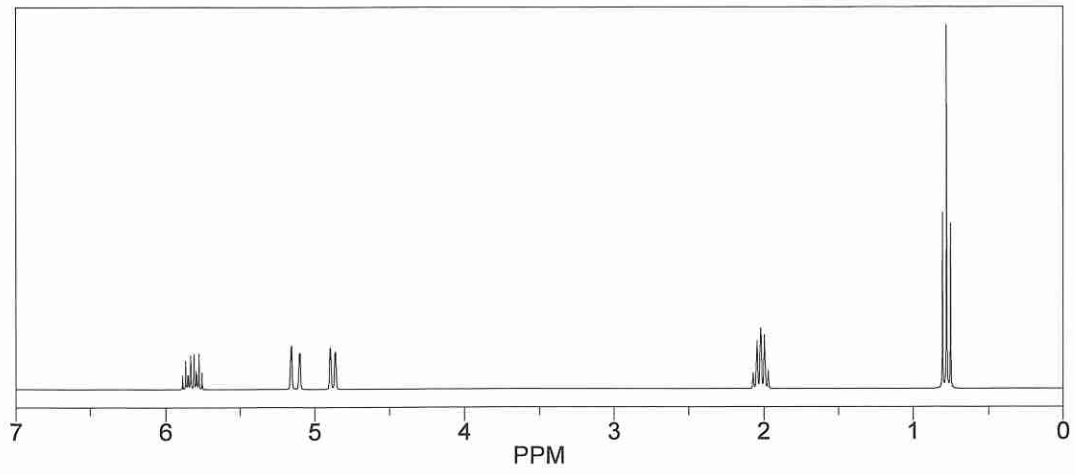
f) R-2-chlorohexane



g) 1,2-dimethylcyclohex-1-ene



h) 1- butene



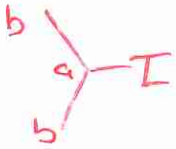
6) What does the n+1 rule mean in proton NMR?

n means neighboring NMR active nuclei (usually a proton). + 1 means you add 1 to get the splitting pattern expected.

7) What does an ethyl group (e.g. ethyl iodide) always look like in the splitting pattern?

a has 3 neighbors so quartet. b has 2 neighbors so triplet.

8) What does an isopropyl group (e.g. 2-iodopropane) look like in the splitting pattern?



a has 6 neighbors so septet

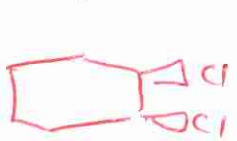
b has 1 neighbor so doublet

9) What determines the coupling constant value?

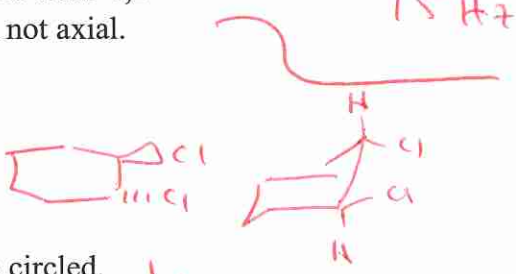
dihedral angle determines coupling constant.

60° is ~ 8 Hz, 90° is 0 Hz (no coupling), 180° is 15 Hz

10) How could you tell whether you had cis-1,2-dichlorocyclohexane or trans-1,2-dichlorocyclohexane? Chlorines are equatorial in the trans isomer and not axial.



for H–H coupling about 8 Hz



larger coupling constant due to larger dihedral angle

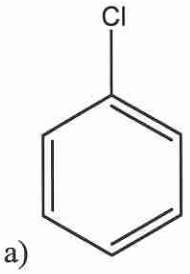
Integration – Integration will be above the peaks if needed and will be circled.

11) Give the integration for the following molecules.

a) Ethane

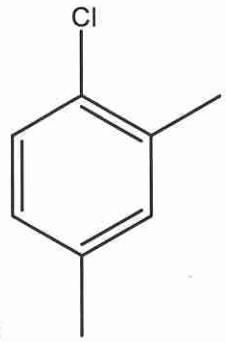
— no integration since only 1 type of hydrogen

FOR AROMATIC BELOW, ASSUME THE AROMATIC PROTONS SHOW UP AS A SINGLET.



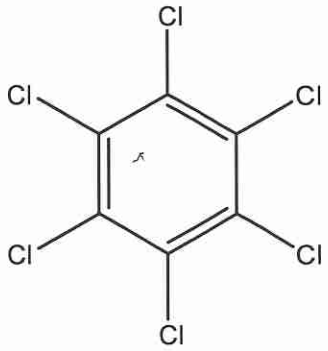
a)

5



b)

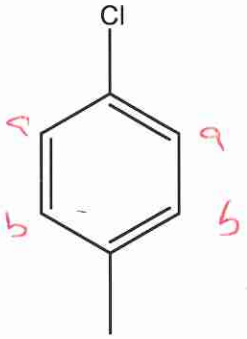
3



c)

0

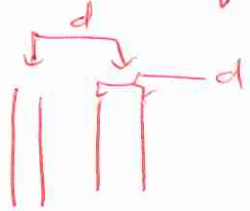
12) Para-disubstitution of benzene is very common in spectra. What would the proton NMR of the following molecule look like?



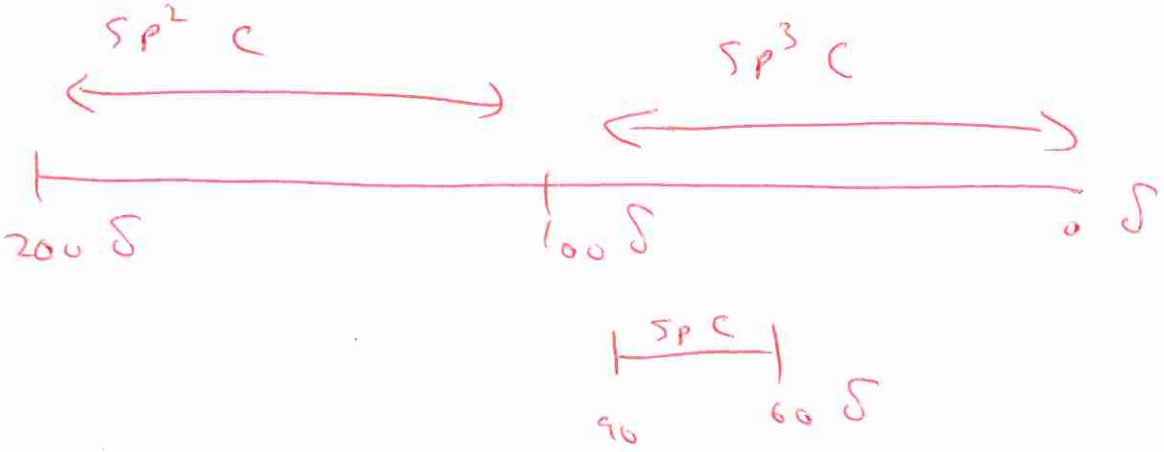
a has 1 neighbor so doublet

b has 1 neighbor so doublet

∴ doublet of doublets



13) Draw the CARBON NMR spectrum from 200 δ to 0 δ. a) Indicate where sp^3 carbons show up relative to TMS. b) Indicate where sp^2 carbons usually show up relative to TMS. c) Indicate where sp carbons up relative to TMS.



14) What does the n+1 rule mean in proton coupled NMR?

n+1 n means number of NMR active nuclei on that carbon CH_3 (quartet) CH_2 (triplet) CH (doublet) C (singlet)