NMR Assignment Workshop: ORGANIC CHEM 4524 Spring 2014

1. Low resolution exercises

a) los res spectra--🡪 molecular structure exercise 8, problem 8.2

b) molecular structure🡪 low res spectra lab exercise NMR-1

 2) High Resolution: rules and exercises

1. Splitting pattern intensities: Pascal triangle lab exercise NMR-2a
2. peak areas: integration curves lab exercise NMR -2a

c) high res spectra🡪 molecular structure lab exercise NMR 2b

3) Clarifications on Lab # 3 assignment

NMR LAB EXERCISE 0 : non-equivalent H count and low resolution spectra to chemical structure

1) how many non- equivalent H do you expect for:

 a) CH3OH (methanol) \_\_\_\_\_

 b) C(CH3)4 (neopentane) \_\_\_\_\_



 c) \_\_\_\_\_

 2-butanol



 d) \_\_\_\_\_\_

 (Z) 3-methyl-2-pentene



e) \_\_\_\_\_\_

 cyclohexane

2) Determine the likely structure of the species below based on their low resolution NMR spectra

C2H6O

C2H6O

C4H8

NMR LAB EXERCISE 1 : molecule🡪 low resolution spectra

Using the attached tables of 1H ppm shifts, sketch the low resolution spectra for the compounds below. Make sure to indicate qualitatively expected relative intensities.



 2 1.5 1 ppm



 5 4 3 ppm



 4 3 2 1 0



 12 9 6 3 0



 5 4 3 2 1

NMR LAB EXERCISE 2-A : high resolution splitting patterns and integration curves

1)Draw the ~ splitting patterns expected for all the non-equivalent H in each compound below and make sure to label which H are creating the given pattern (You can consult the `Pascal Triangle’ below)

2)Sketch the expected integration pattern if it is collected from high to low ppm.



 2 1.5 1



*for > 6 NN, just sketch ~ # lines*

 2 1.5 1 0.5



 5 4 3 2 1



 4 3 2 1 0

  *NN=#nearest neighbors*

 1 0

Pascal’s triangle

1. 1 1

 1 2 1 2

 1 3 3 1 3

 1 4 6 4 1 4

 1 5 10 10 5 1 5

 1 6 15 20 15 6 1 6

NMR LAB EXERCISE 2-B: high resolution spectra🡪 structure

Sketch the molecular structure and assign H to the various peaks a🡪c



C3H8O (HINT: not an alcohol) MOLECULAR STRUCTURE



b

a

c

C7H8

unresolved multiplet



relative intensities:

a:b:c;d =1:1:3:3

B = octuplet

 c d

 a b

C4H8O (hint: note that peak *a* is at ~9.5.

Only one commonly occurring H does that: HC=O)

C3H5Cl3



 4 3 2.5

c

b expanded

b

a

b

a