**Chem 4524 Spring 2016 Organic Chemistry II**

NMR lab Dry Lab Assignment #1: 1H NMR Molecular Structures

Alfred State College

Your name:\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_answers\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

* 1. The following compounds have only a singlet NMR signal at the indicated δ vs TMS. Draw the structure

 of the molecule implied by the simple NMR spectrum observed. (2 pts each, 6 pts total)



1. C8H18 δ=0.9 singlet
2. C5H10 δ=1.5 singlet



 

Equivalent H don’t split each other

 c) C8H18 O δ =2.2 singlet



1.2 Deduce and draw the molecular structure of the organic compounds based on the 1H NMR spectra and molecular formulas provided below. (3 pts each, 15 pts total)

1. C6H12 B E

H site

A

B

C

D

E

 

C D A

|  |  |  |
| --- | --- | --- |
| δ vs TMS | Splitting count | #H |
| 0.9 | 3 | 3 |
|  1.6 | 1 | 3 |
| 1.7 | 1 | 3 |
| 2.0 | 5 | 2 |
| 5.1 | 3 | 1 |





1. C4H6Cl4

H site

a

b

|  |  |  |
| --- | --- | --- |
|  δ vs TMS | Splitting count | #H |
| 3.9 | 2 | 4 |
| 4.6 | 3 | 2 |

 b a a b a b b a

several choices (first one slightly less so based on δ)

1. C4H6Cl2

x



y

H site

x

y

z

x

z

|  |  |  |
| --- | --- | --- |
|  δ vs TMS | Splitting count | #Hy |
| 2.2 | 1 | 3 |
| 4.1 | 2 | 2z |
| 5.7 | 3 | 1 |

1. C5H10O

H site

a

b

c

b

a

c



|  |  |  |
| --- | --- | --- |
|  δ vs TMS | Splitting count | #H |
| 1.0 | 2 | 6 |
| 1.3 | 7 | 1 |
| 2.3 | 1 | 3 |

1. C3H8O

y

x x

 z

H site

x

y

z

|  |  |  |
| --- | --- | --- |
|  δ vs TMS | Splitting count | #H |
| 1.1 | 2 | 6 |
| 3.3  | 1 (broad) | 1 |
| 3.8  | 7 | 1 |

1.3. The observed NMR for compound X with the formula C8H10 O is below.

1. Assuming it is an alcohol what is the likely organic structure of the compound ? (note that the

 peaks at 4.9 and 1.6 are expanded to show splitting in insets. (2 pts)

 c



d

 b

a

d

b

c

 Compound X’s molecular structure

a

1. Label the non-equivalent H in X’s structure with their NMR signal a🡪d (2 pts)