**Laboratory #4: NMR Dry Lab #2 assignment**

**13C and Molecular Assignment from Real Spectra**

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

**Textbook 13C NMR Assignments**

13C NMR is even more convenient than 1H NMR in that the former yields only singlets and a signal for each non-equivalent C in a structure. Use this simple fact to assign the molecular structure for the C6H14 isomer based on the listed 13C NMR below:

2 pts 2 pts



a b c

**δ 13.7 CH3 a δ 8.5 CH3 a b**

**δ 22.8 CH2 b**  **δ 28.7 CH3  b c d**

**δ 31.9 CH2 c  δ 30.2 C c**

**δ 36.5 CH2  d**

**a**

Determine the structure of the C4H10O isomers below based on their listed 13C NMR data



**δ 18.9 CH3 a δ 10 CH­3 a b**



**δ 30.8 CH b δ 22.7 CH3 b a c d**

**δ 69.4 CH2 c c δ 32.0 CH2 c**

**b a δ 69.2 CH d**

**Compound X =**

**a b**



**Think benzene ring**

**CH b c CH3 a**

**C c**

135 131 20 ppm

The above 13C NMR spectrum is recorded for a compound X with the molecular formula C10H14.

Draw its likely structure of X in the box provided.

**detailed answers to structures: C7H8O2 and C8H10**

#1) **3- methoxyphenol C7H8O2**

* Has 7 unique carbons consistent with 13-C NMR
* Strong OH band at 3350 cm-1 and C=C breathing mode at 1600 cm-1
* Splittings match: X doublet most down field near OCH3; Y doublet less down field since further from OCH3 and OH, and is obscured slightly by singlet Z
* No methylene stretch at 1470 cm-1 … all methyl



d

(singlet,3H)

X doublet `

Z singlet

a- triplet c

Y doublet

(one peak obscured by Z singlet)

**#2) Meta xylene C8H10**

* Has 5 unique carbons out of 8 total. Methyls are identical and carbons in ring next to methyl-bearing C are the same
* All H assignments consistent with splitting and H count (b region is sum of doublet and singlet)
* IR stretch above 3000 cm-1 with overtones at 2000, 1600 and 1500 cm-1=> aromatic ring
* Only 1370 cm‑1 methyl bend present

b (doublet, 2H)



c (singlet H of methyls)

b (larger singlet between doublet, 1H)

c (singlet H of methyls)

a (triplet, 1H)

b (doublet, 2H)