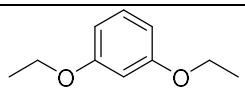
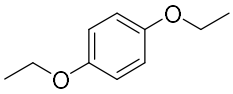
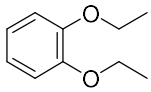
Name:

Student #

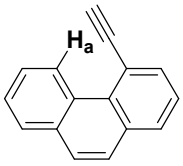
Monday, Novembre 23, 2015

CHM 3122 – Quiz 2
(Stage 1; duration: 20 min)
Applications of Spectroscopy in Chemistry

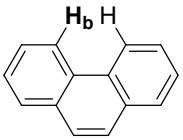
1) Predict the number of signals (peaks) expected for these following structures in these different types of experiments: ^{1}H NMR, ^{13}C NMR, DEPT-135, DEPT-90 et DEPT-45 : (**15 points**) **(1pt each)**

Structures	^{1}H NMR	^{13}C NMR	DEPT-135	DEPT-90	DEPT-45
	5	6	5	3	5
	3	4	3	1	3
	4	5	4	2	4

2) Which proton will be the most deshielded in these two structures: **H_a** from structure **I** or **H_b** from structure **II**? Why? (**10 points**)



I



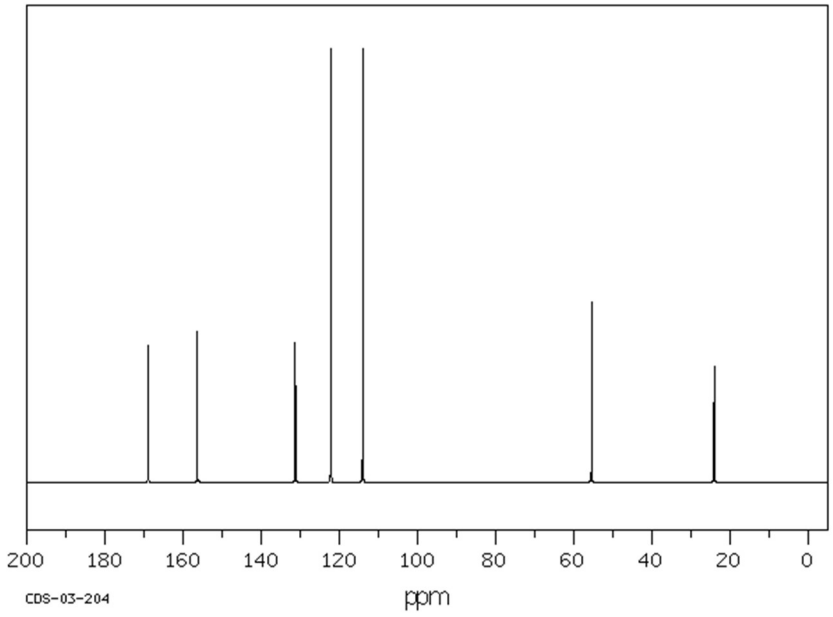
II

H_a from structure **I** is the most deshielded **(4 pts).**
Magnetic anisotropy effect from alkyne **(3pts).**
H_a is in the deshielding zone of alkyne or you can refer to it as the region (-) from the shielding cones of the alkyne. In other words, it is in the induced magnetic line that is aligned with the external magnetic field B_0 **(3pts).**

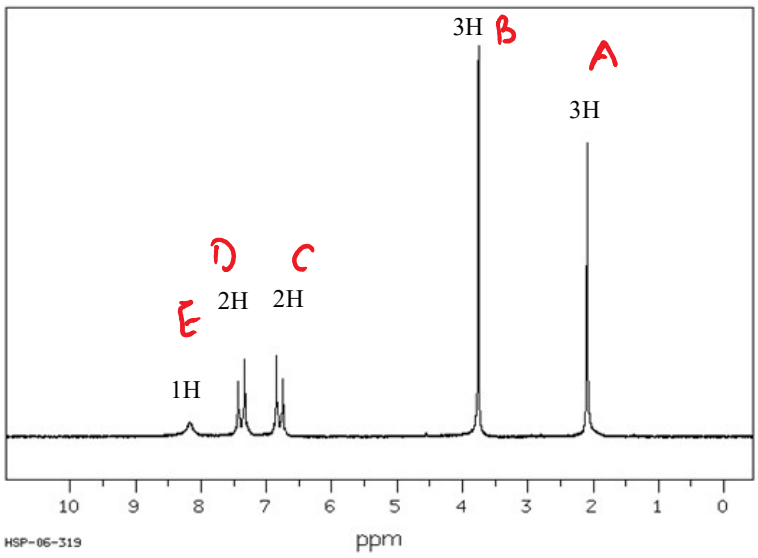
3) Determine the structure of this compound with molecular formula $C_9H_{11}NO_2$ using the carbon-13 and proton spectra below. The carbon-13 and the DEPT experimental results are also tabulated. *Questions that follow are to guide you in your answer.* (**25 points**):

a) What is the degree of unsaturation? Show your calculations. (**2 points**)
DU = 2C+2-H-X+N/2 = 18+2-11-0+1/2 = **5**

b) Fill in the following tables: (**10 points**)



Normal Carbon	DEPT-135	DEPT-90	Resultts (0.5 pt each)
24.1 ppm	Positive	No peaks	CH_3
55.4	Positive	No peaks	CH_3
114.0	Positive	Positive	CH
122.2	Positive	Positive	CH_3
131.3	No peaks	No peaks	C
156.4	No peaks	No peaks	C
168.9	No peaks	No peaks	C



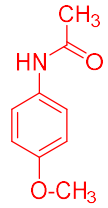
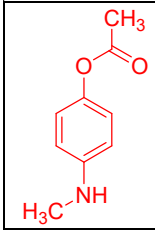
Signal	δ (ppm)	Integration	Multiplicity	Comments (6.5 pts total)
A (1.5pt)	2.05	3	s	CH_3 next to C // δ(ppm) next to C=O
B (1.5pt)	3.85	3	s	CH_3 next to O, C or N // δ(ppm) next to O
C (1pt)	6.83	2	d	para-substituted benzene; symmetry; 2 doublets where each integrates to 2H.
D (1pt)	7.45	2	d	
E (1.5pt)	8.18	1	brs	NH (broad singlet)

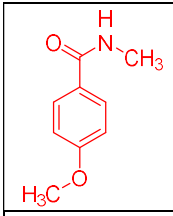
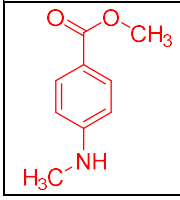
c) Present the different fragments found in the table: (**5 points**)

Fragments	  O-CH_3 NH

d) Draw the final structure of the compound. (Show briefly your reasoning) (**8 points**)

Possibilities:

	the correct structure because C=O is 168.9 ppm of an ester or amide and not ketone (8pts)
	Partially acceptable structure because there's a difference in chemical shifts of a methyl next to NH which is around 3-3.5 ppm and the one next to O is around 3.5-4.5 ppm due to the more electronegativity effect of O (7pts)

	Partially acceptable structure because none of the methyls in this structure will have a chemical shift around 2 ppm because of the electronegative effect of N or O (7pts)
	Partially acceptable structure because none of the methyls in this structure will have a chemical shift around 2 ppm because of the electronegative effect of N or O (6pts)