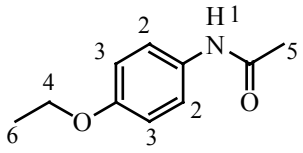
HW #2 Answer Key March 1

1. Chemically distinguishable environments for $C_5H_{11}Cl$

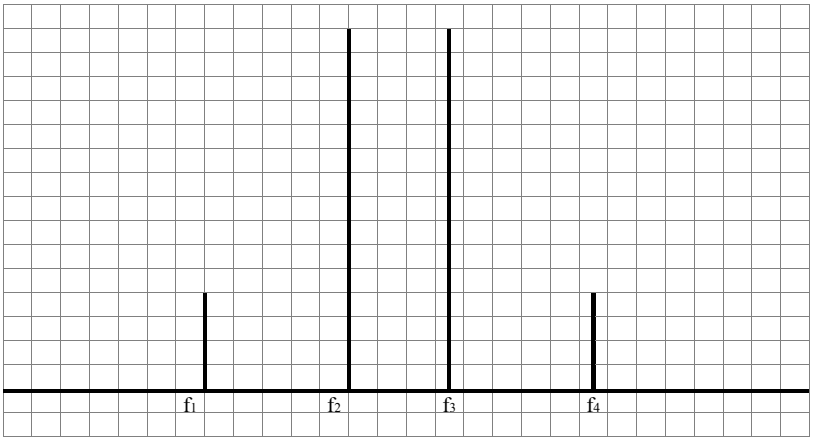
Isomers	^{13}C Spectrum	^{1}H Spectrum
chloropentane	5	5
2-chloropentane	5	5
3-chloropentane	3	3
2-methyl-1-chlorobutane	5	5
2-methyl-2-chlorobutane	4	3
2-methyl-3-chlorobutane	4	4
2-methylchlorobutane	4	4
2,2-dimethylchloropropane	3	2

2. $C_{10}H_{13}NO_2$: para ethoxyl phenyl ethyl amide



Assignment	1	2	3	4	5	6
Shift (ppm)	7.94	7.36	6.80	3.98	2.09	1.38

3. (a) $\nu_A - \nu_B = \sqrt{20 \cdot 10} = 14\,\text{Hz},\ J_{AB} = 5\,\text{Hz}$
At half of the applied field, the chemical shift difference should decrease to one-half $\nu_A - \nu_B = 7$ Hz, while *J*-coupling stays the same $J_{AB} = 5\,\text{Hz}$.



The solutions for the combination

$$\Delta\nu = [(f_1 - f_4)(f_2 - f_3)]^{1/2} = 7 \text{ Hz}$$

$$J = f_1 - f_2 = f_3 - f_4 = 5 \text{ Hz}$$

$$\frac{I_2}{I_1} = \frac{I_3}{I_4} = \frac{|f_1 - f_4|}{|f_2 - f_3|}$$

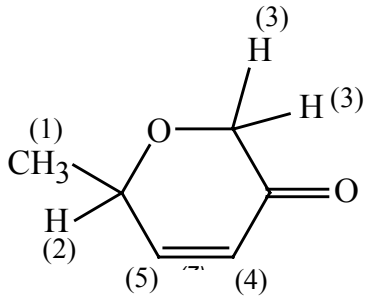
are $f_2 - f_3 = 5\sqrt{3} - 5 = 3.66$ Hz and $I_2/I_1 = 2 + \sqrt{3} = 3.73$

(b) Because the lines are evenly spaced and the ratio of the intensities is 1:3:3:1, it could be either a proton coupled to a methyl group, or an AB spin pair with their J coupling constant being exactly $1/\sqrt{3}$ of their chemical shift difference in Hz unit at this external field. If it's coupling to methyl group, the pattern should not change with changing external field; for AB spin pair, the spacing between the center two lines will increase with increasing external field.

4. The proton connected to the same carbon as the methyl group is H_A, because ${}^3J$ is larger than ${}^4J$.

ν_A	ν_M	ν_X	${}^3J_{AM}$	${}^3J_{AX}$	${}^4J_{MX}$
7.1 ppm	5.85 ppm	1.92 ppm	16 Hz	7 Hz	2 Hz

5.



Assignment	1	2	3	4	5
Shift (ppm)	1.4	3.8	4.2	6.1	6.9