

Organic Chemistry: CHEM 231B

Whittier College

Spring 2004

Problem Set #1

Due Thursday 2/19/2004 @ 12:00 p.m.

40 pts

1. Consider the following experimental results: (17 pts)

If (2R) 1-phenyl-butan-2-ol is treated with trifluoromethylsulfonyl chloride and pyridine in dichloromethane, a single product is isolated following the reaction and workup. The $^1\text{H-NMR}$ of product is nearly identical to the starting material; the IR reveals the loss of a strong broad peak between $3150 - 3475 \text{ cm}^{-1}$ and the formation of two new peaks at 1395 cm^{-1} and 1180 cm^{-1} . Upon treatment of this compound with t-butoxide in tetrahydrofuran, GC-MS analysis reveals one major peaks and three minor peaks, all of which have a M^+ peak = 132 m/z. IR analysis of the complex mixture reveals the loss of several peaks including peaks at 1395, 1210, and 1180 cm^{-1} peaks and the formation of several new peaks near 3030, 1620, 990 and 675 cm^{-1} .

- 1a. What are the four products? (2 pts)
1b. How would you use NMR to determine the identity of the major peak? Be explicit!!! (8 pts)
1c. Of all the spectral possibilities for each product, what single NMR peak for each product would be the most characteristic for determining the identity of the major product? Explain. (5 pts)
1d. Which product do you think would be the major product and why? (2 pt)

2. See attached pages of problem set for questions about the spectral data. (15 pts)

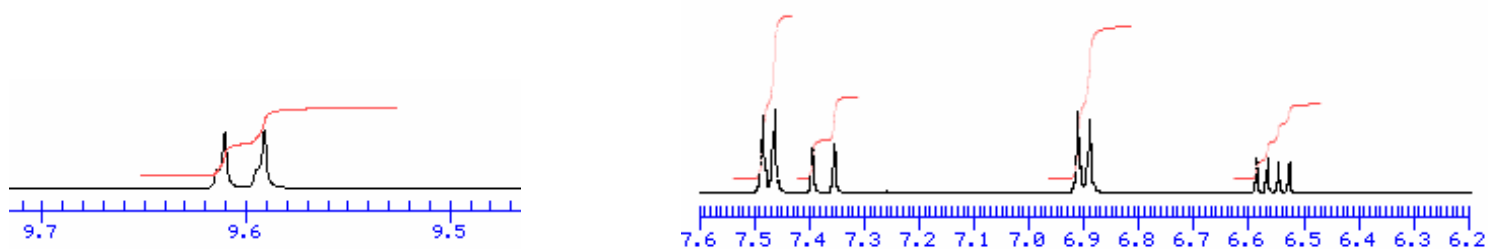
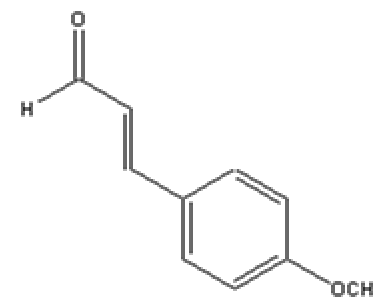
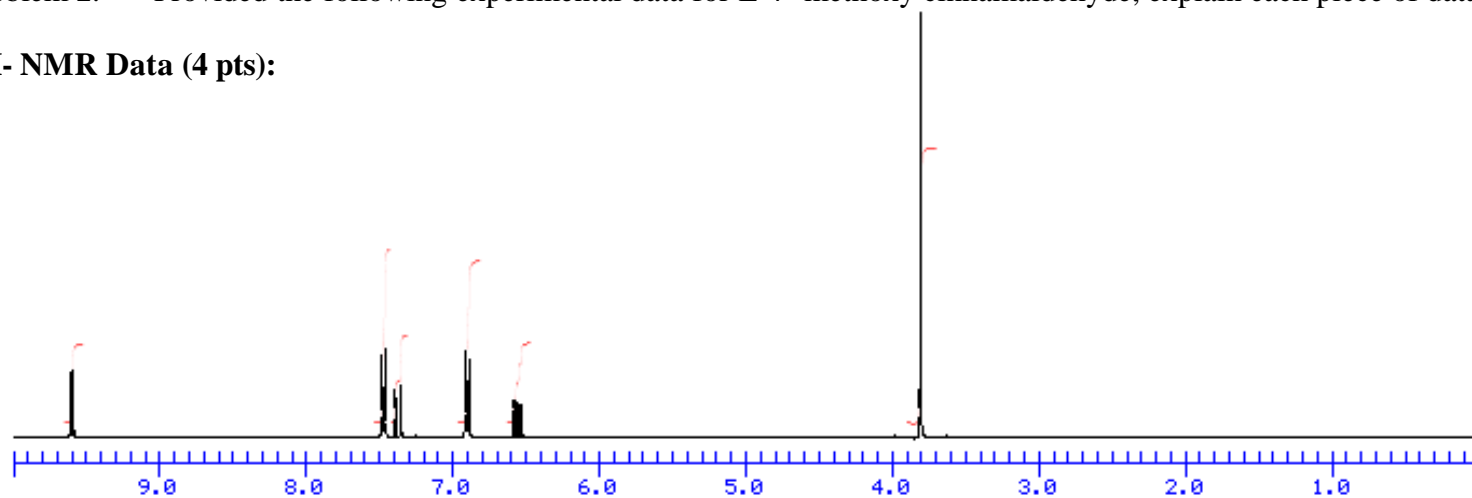
3. Consider the following series of experiments: (9 pts)

Compound A, C_6H_{10} , reacts with H_2 in the presence of Pd / C to give methylcyclopentane. In subsequent reactions, if Compound A reacts with either mercuric acetate in water followed by sodium borohydride OR with Borane-THF followed by peroxide in aqueous sodium hydroxide OR with aqueous HCl, only one product, compound B, is produced.

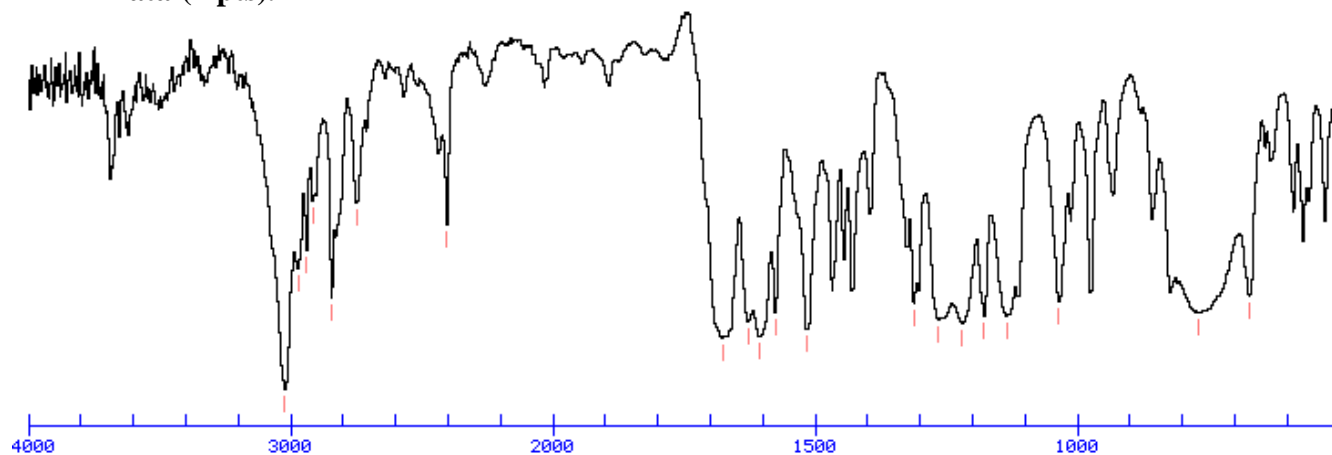
- 3a. Propose structures for compounds A & B. (4 pts)
3b. Provide mechanisms for the formation of B using two of the three reactions (4 pts)

Problem 2. Provided the following experimental data for E 4'-methoxy cinnamaldehyde, explain each piece of data completely.

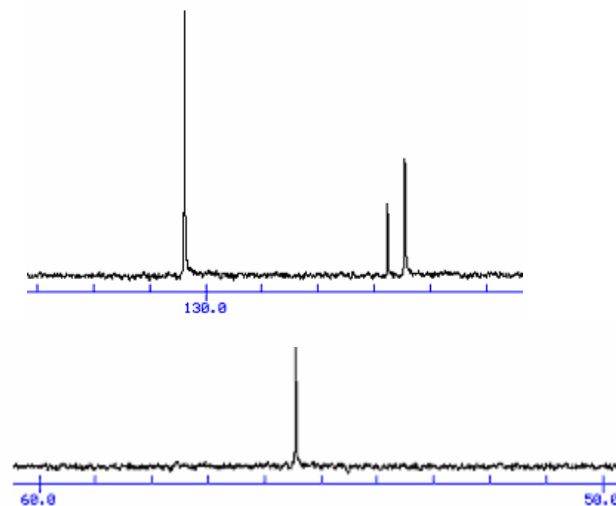
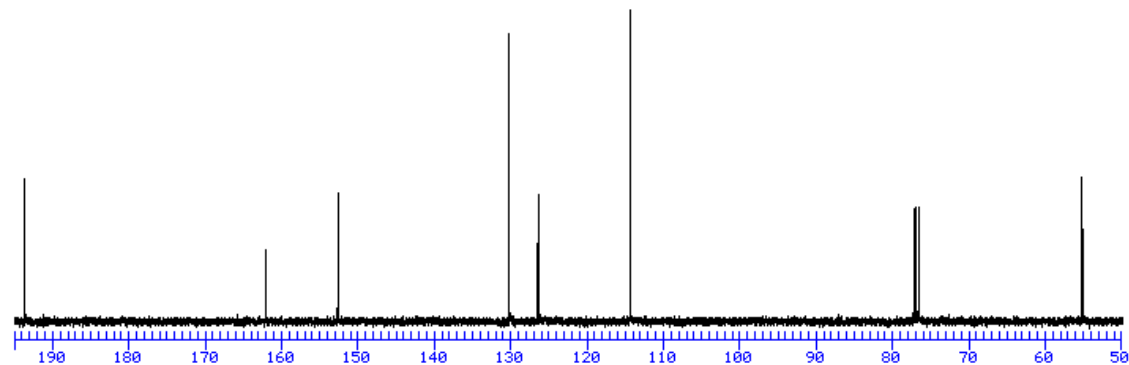
¹H- NMR Data (4 pts):



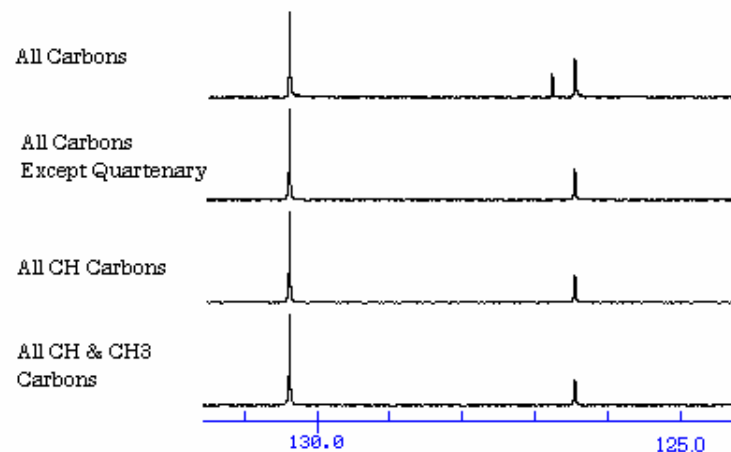
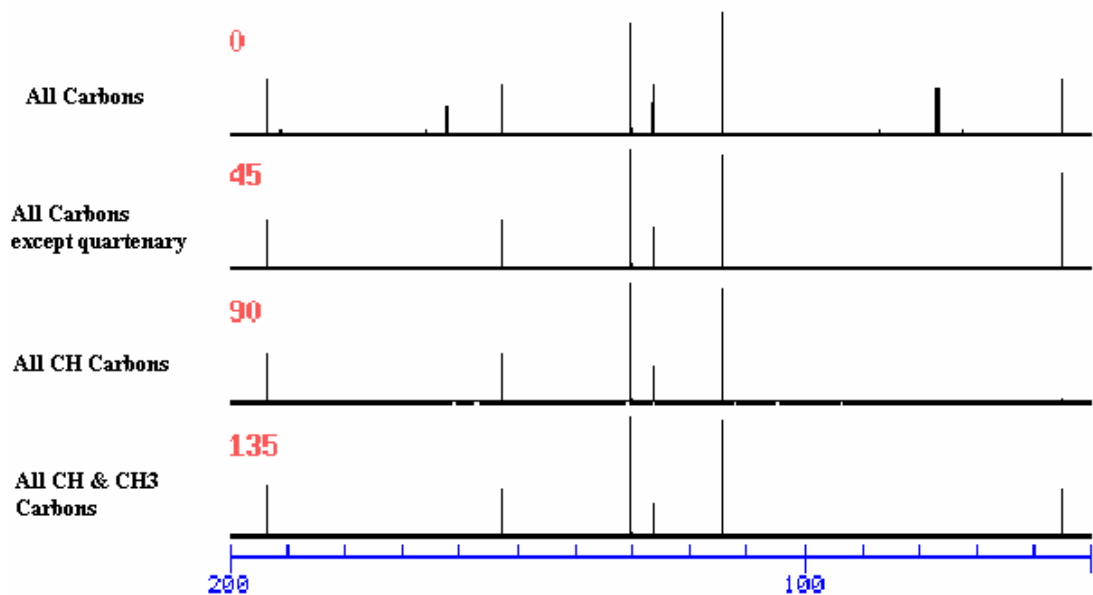
FT-IR Data (2 pts):



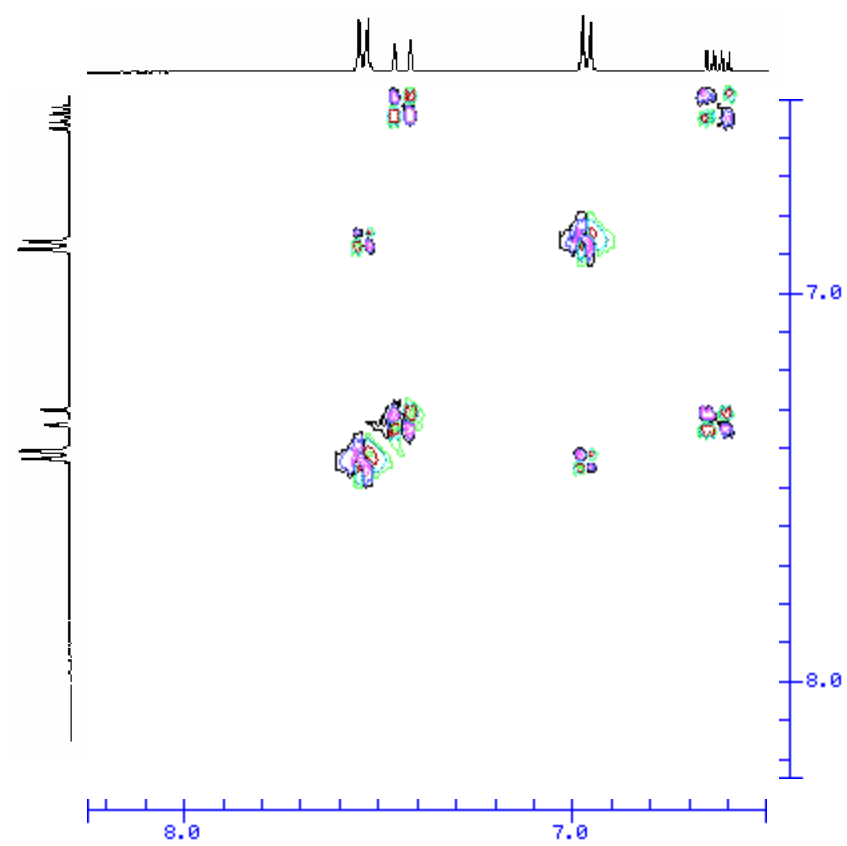
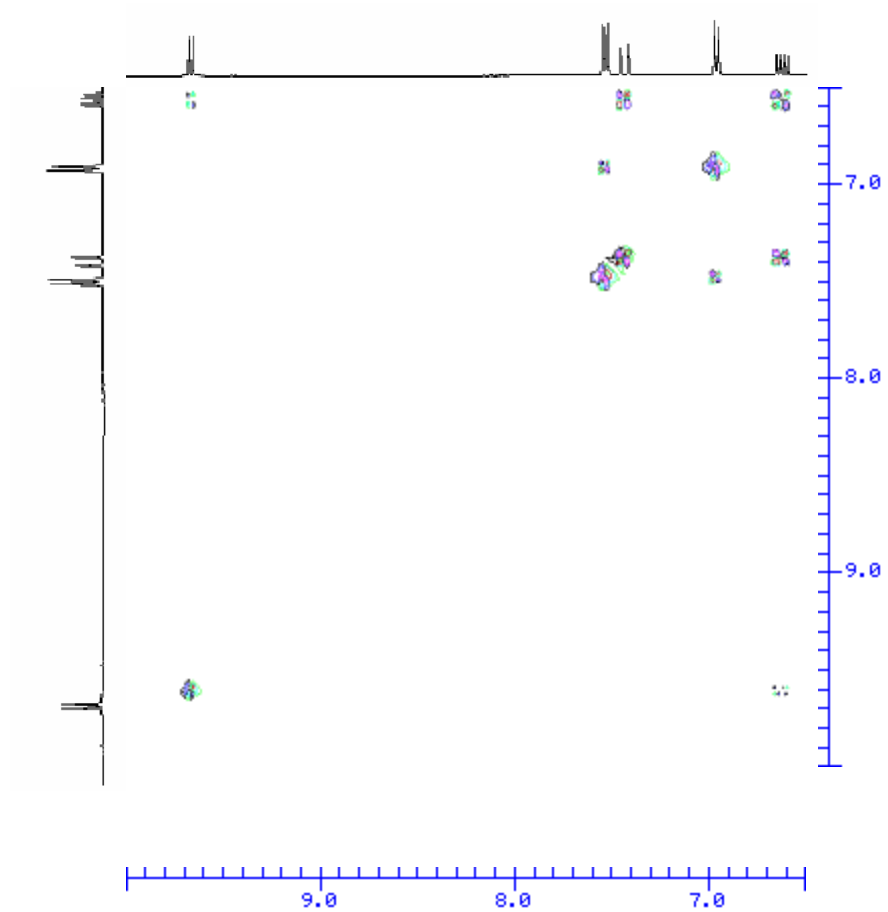
¹³C- NMR Data (3 peaks at 77 are from solvent– CDCl₃) (3 pts)



DEPT Spectra (the “all carbon” spectra is the same as above) (3 pts)

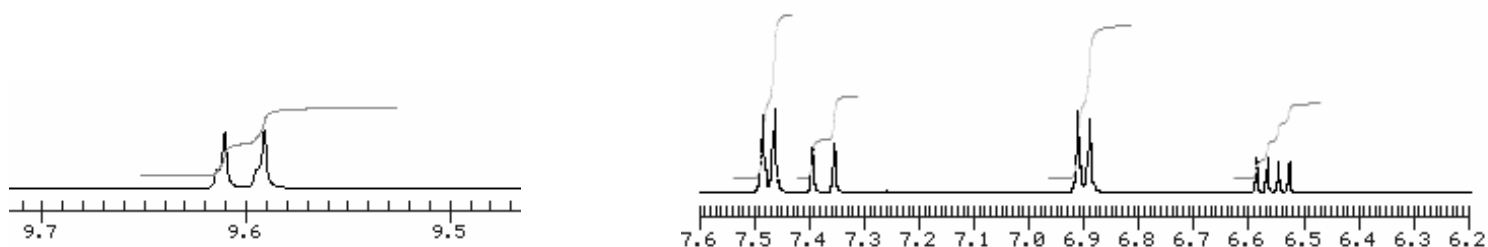
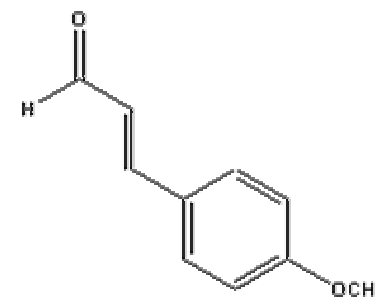
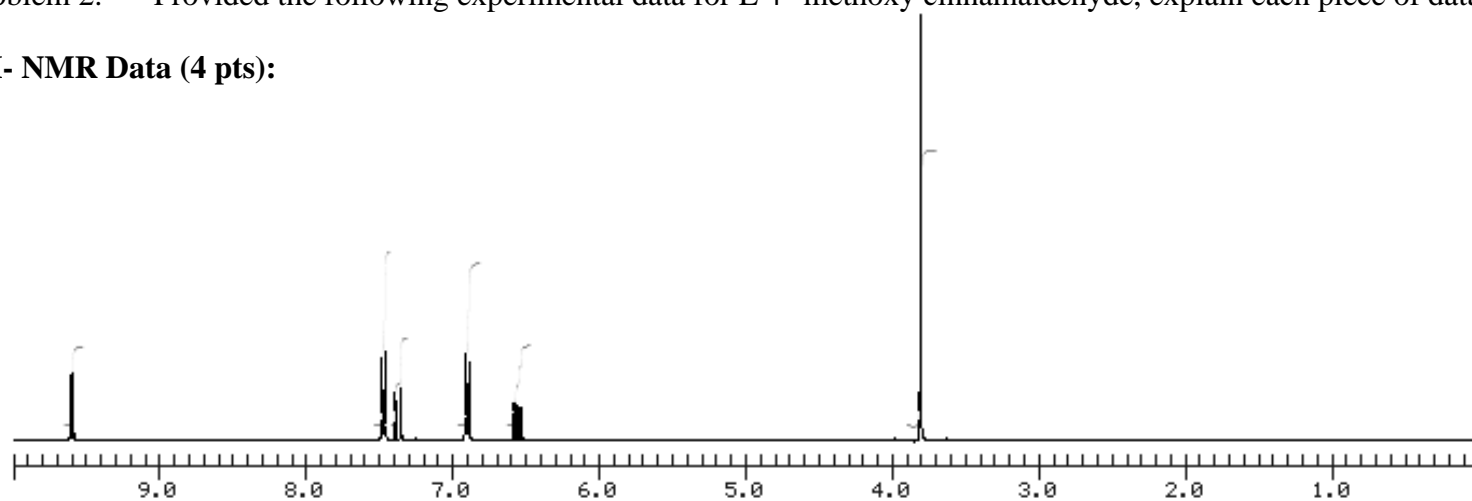


COSY Spectra (spectra are zoomed in and ignore the peak at 3.8 ppm, which has no off-axis peaks) (3 pts)

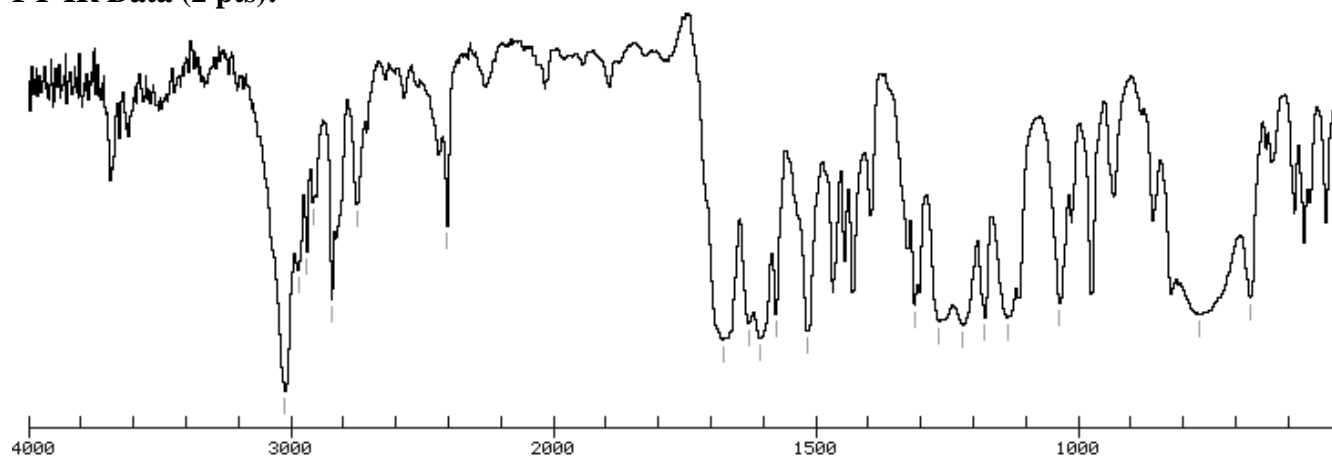


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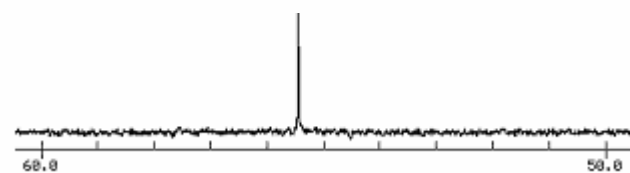
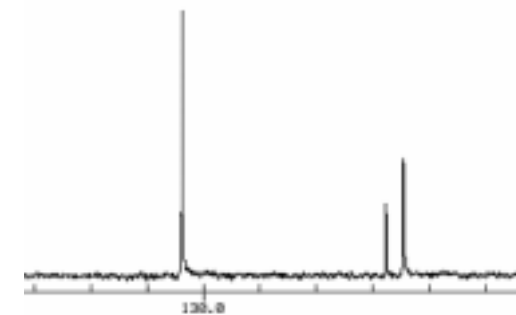
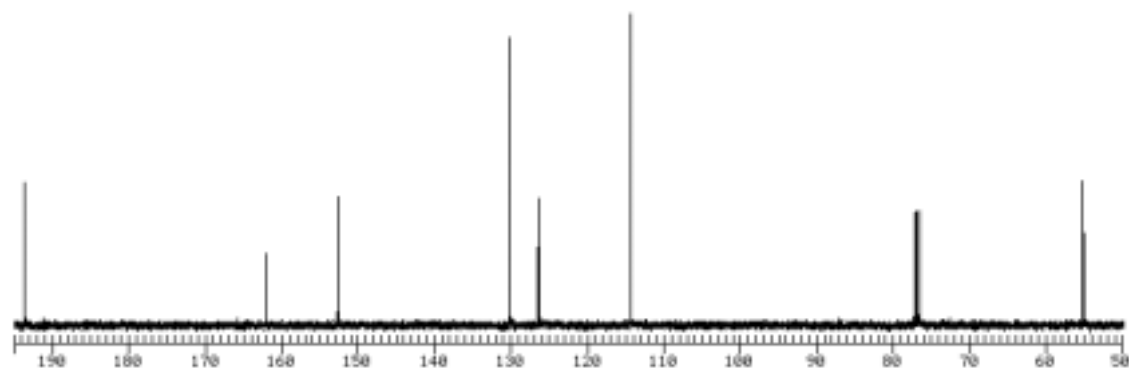
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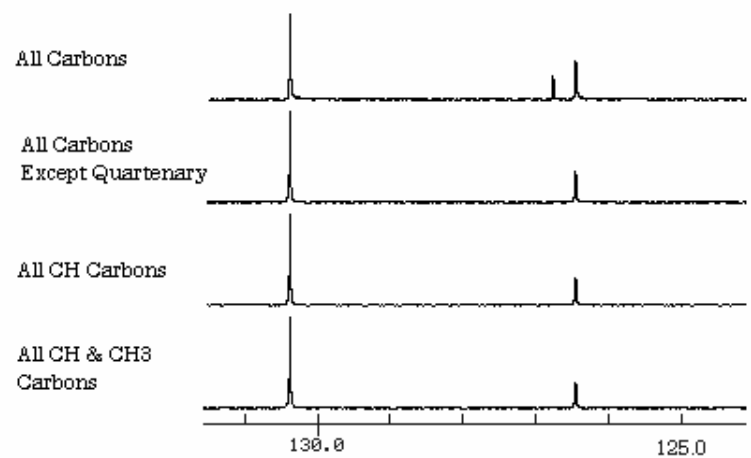
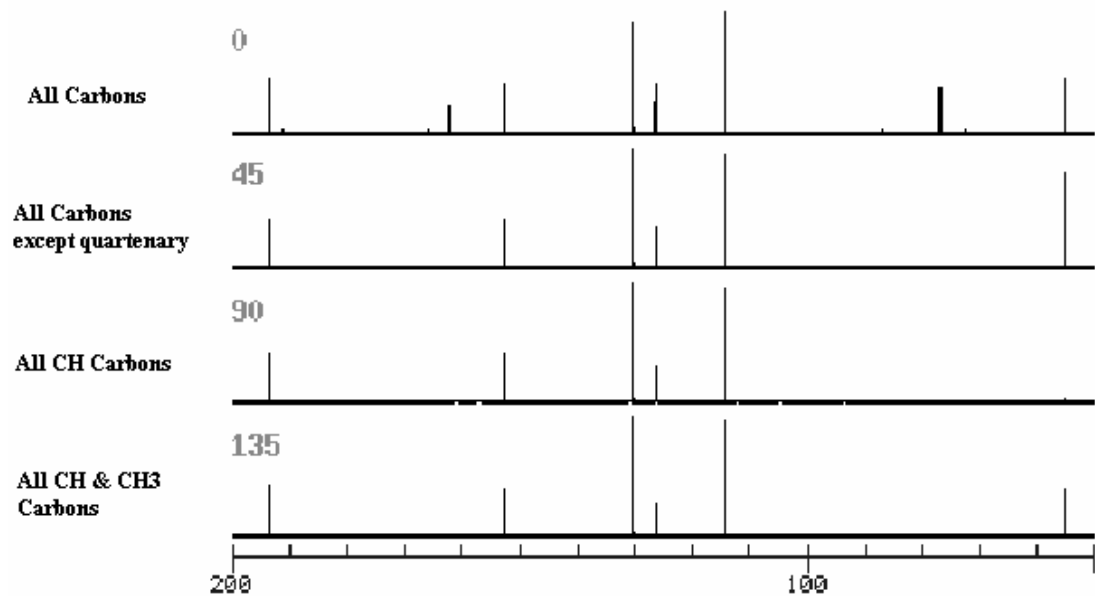
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