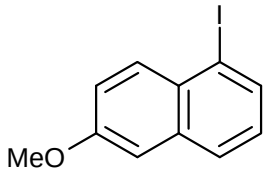
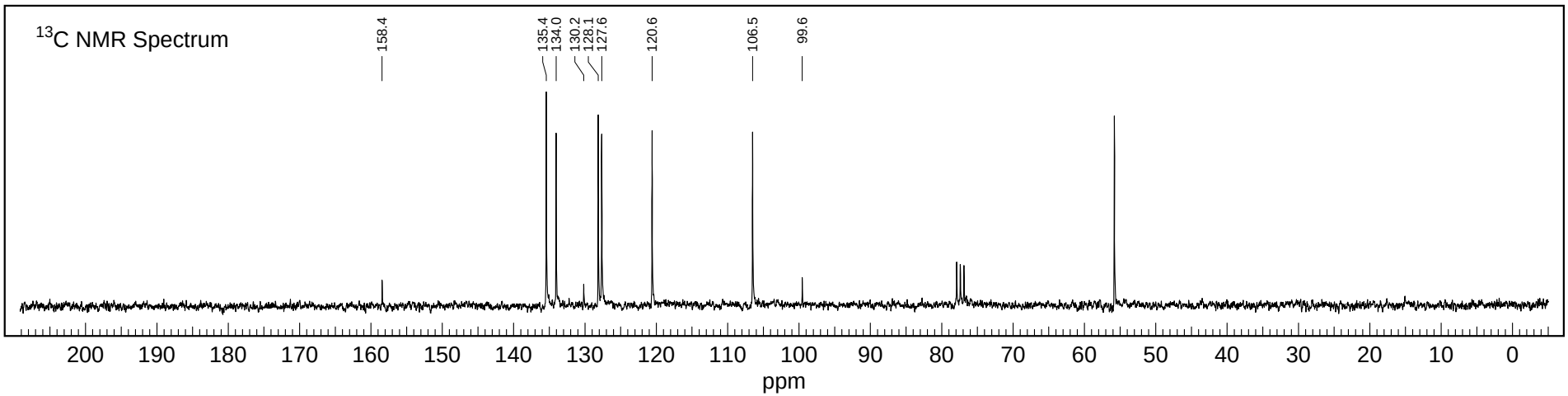
Problem R-11E ($C_{11}H_9IO$)

250 MHz ^{1}H NMR Spectrum in $CDCl_3$

Source: Adam Fiedler/Reich

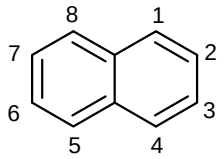


^{13}C NMR Spectrum



PLT ex-1-2011-12-gq.plt

Problem R-11E ($C_{11}H_9IO$). You are provided the ^1H NMR spectrum of a disubstituted naphthalene (**the substituents are methoxy and iodo**). You are required to analyze the NMR spectrum, and determine the structure or structures.



(a) For each of the 8 positions on the naphthalene as defined above, give either the substituent at that position, or the NMR signal (δ, multiplicity and J values). If there is more than one plausible structure assignment, draw the alternative structure, and indicate your preference. To make grading easier, **please place the methoxy substituent at either 1 or 2**.

1_____

2 _____

3 _____

4 _____

5 _____

6 _____

7 _____

8 _____

(b) Briefly describe the key evidence that led to your structure assignment.

20

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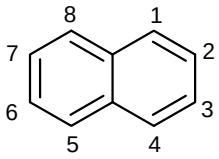

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8

1 7.03, d, J = 2.5 Hz

2 **OCH_3**

3 7.19, dd, J = 9, 2.5 Hz

4 7.97. d (t), J = 9 (<1) Hz

5 **I**

6 7.90, dd, J = 7.5, 1.5

7 7.07, dd, J = 8, 7,5

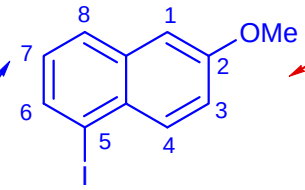
8 7.68, d(t), J = 8 (~1) Hz

key multiplet

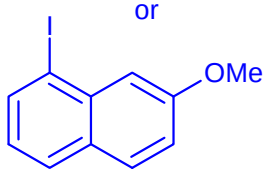
key multiplet

10 points for considering both

8 points for one or the other



or



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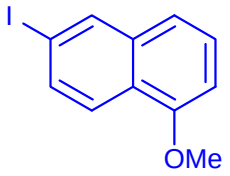
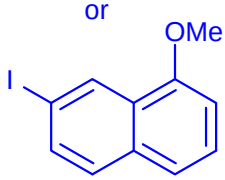
6 points for one or the other

(See item 2 below)



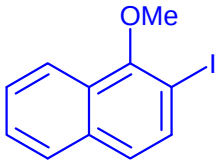
or



(b) Briefly describe the key evidence that led to your structure assignment.

2

1. The substituents must be in different rings, otherwise would see two td (o,o,m) from protons in the unsubstituted ring



2. The d (J=2.3 Hz) at 7.03 means that one substituent must be at a β position, the upfield shift means this is ortho to OMe (δ_o = -0.45 in benzene, -0.7 in naphthalene)

3. The big dd (J = 8, 7.5) means the other substituent has to be at peri position (5 or 8). Deciding among these is hard, since only long-rang couplings distinguish them.

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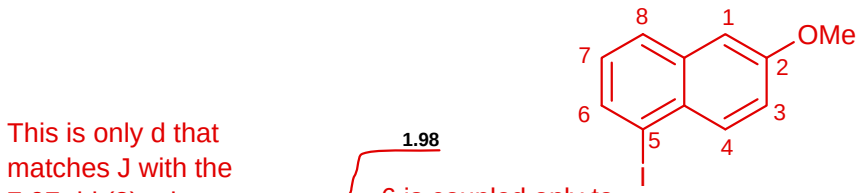
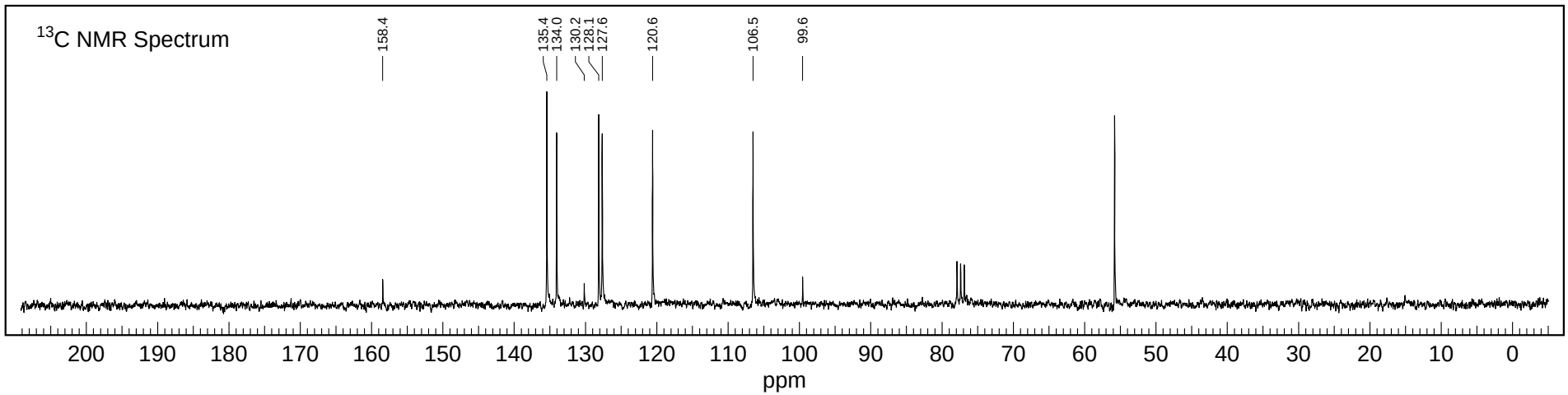


This is only d that matches J with the 7.07 dd (3) - thus this is 4

6 is coupled only to 7 and 8 - no other long range coupling

8 has more long-range coupling opportunities (to 4 and 1)



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