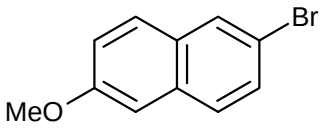
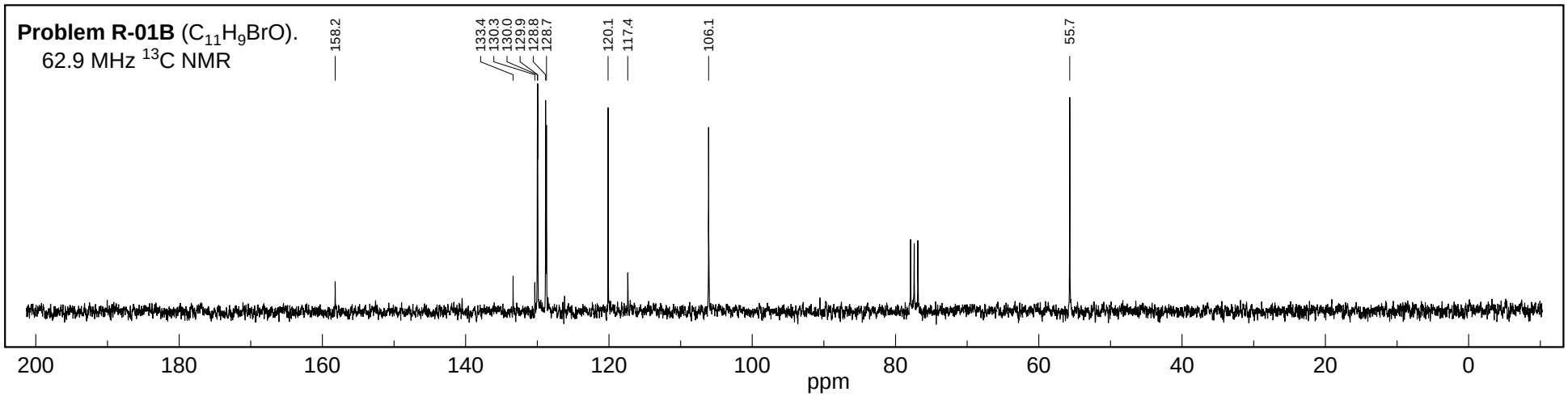
Problem R-01B ($C_{11}H_9BrO$).
250 MHz ^{1}H NMR Spectrum in $CDCl_3$.
Source: Adam Fiedler/Reich 10/29 g

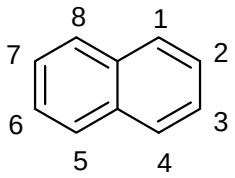


Problem R-01B ($C_{11}H_9BrO$).
62.9 MHz ^{13}C NMR



PLT ex-1-2001-g.plt

Problem R-01B ($C_{11}H_9BrO$). You are provided the ^1H NMR spectrum of a disubstituted naphthalene (the substituents are **methoxy** and **bromo**). Your task is 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 asignment, draw the alternative structure, and indicate your preference. To make grading easier, please place the methoxy substituent at either 1 or 2. You may assume that naphthalene NMR properties are similar to those of benzene.

1 _____

2 _____

3 _____

4 _____

5 _____

6 _____

7 _____

8 _____

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

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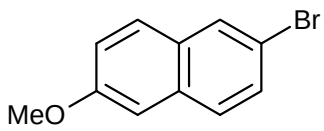

PLT ex-1-2001-g.plt

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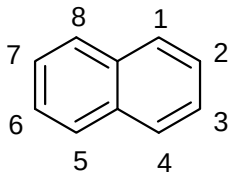


(a) For each of the 8 positions on the naphthalene as defined above, give either the substituent at that position, or the NMR signal (δ , multiplicity and *J* values). If there is more than one plausible structure asignment, draw the alternative structure, and indicate your preference. To make grading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

1 δ 7.07, d, *J* = 2.4 Hz

2 OMe

3 δ 7.14, dd, *J* = 8.8, 2.4 Hz

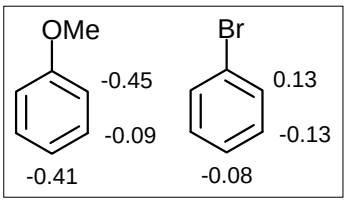
4 δ 7.62, d, *J* = 9 Hz

5 δ 7.89, d, *J* = 1.8 Hz

6 Br

7 δ 7.48, dd, *J* = 8.8, 1.8 Hz

8 δ 7.58, d, *J* = 9 Hz



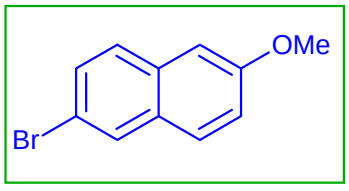
These two are upfield - probably ortho and/or para to OMe. They are coupled to each other by 2.4 Hz (meta), from leaning of the small coupling.

These couplings, together with the d at 7.62, require a 1,3,4-relationship between the protons on the OMe-substituted ring, so substituent must be at 2-position

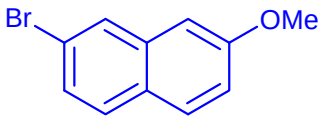
The multiplets at 7.89 (small d), 7.48 (dd) and 7.58 (large d) also require a 1,3,4-relationship of the protons, so the Br subsituent is on the other ring, and at the 6 or 7 position

The 2 superimposed doublets at 7.58 (H^8) and 7.62 (H^4) (could be mistaken for a triplet) are not simple to distinguish, but the leaning of the 7.48 peaks favors the assignment given.

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



or



Hard to distinguish these two isomers - probably an NOE experiment would give useful information - there would be NOE cross-peaks between the 1,8 protons, and the 4,5-protons.

Problem R-01B ($C_{11}H_9BrO$).
250 MHz ^{1}H NMR Spectrum in $CDCl_3$.
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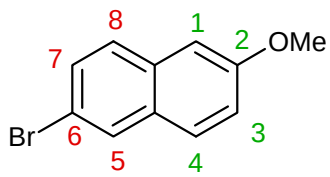

PLT ex-1-2001-g.plt