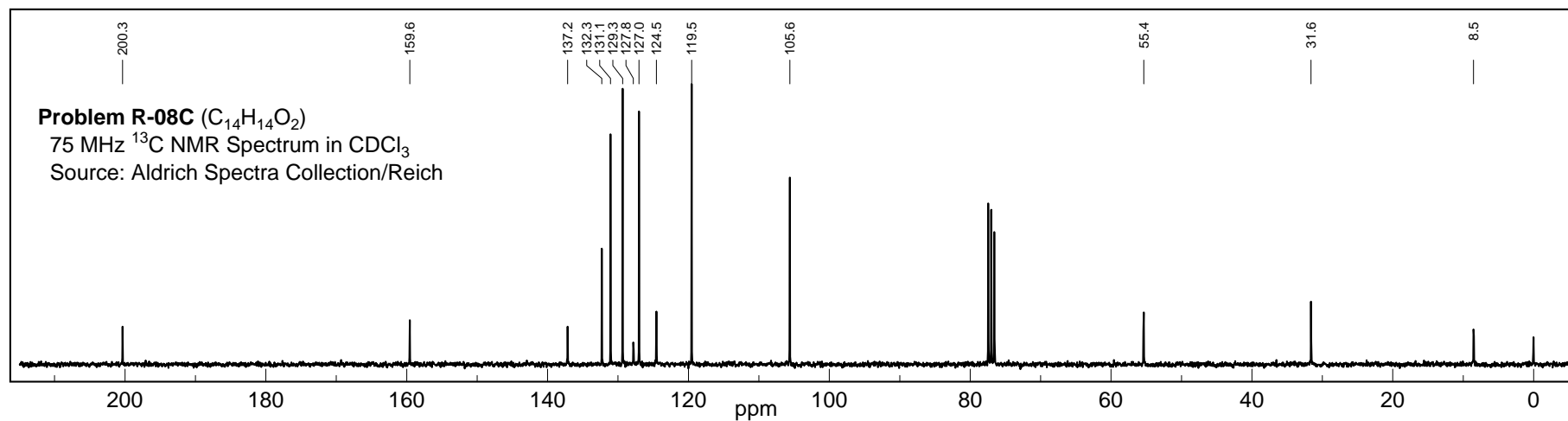
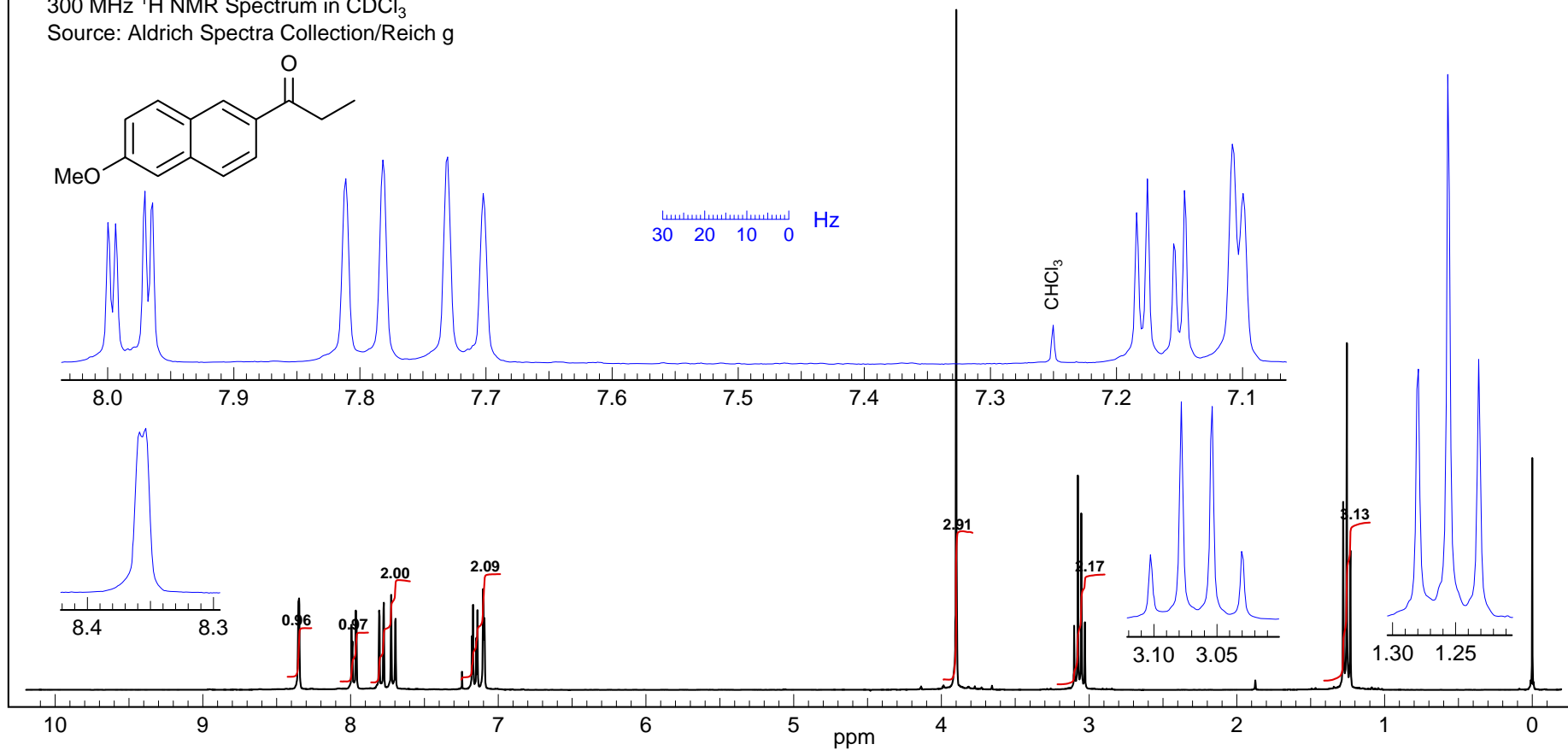
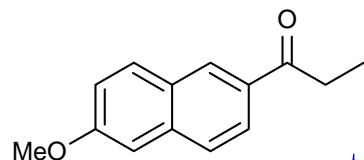
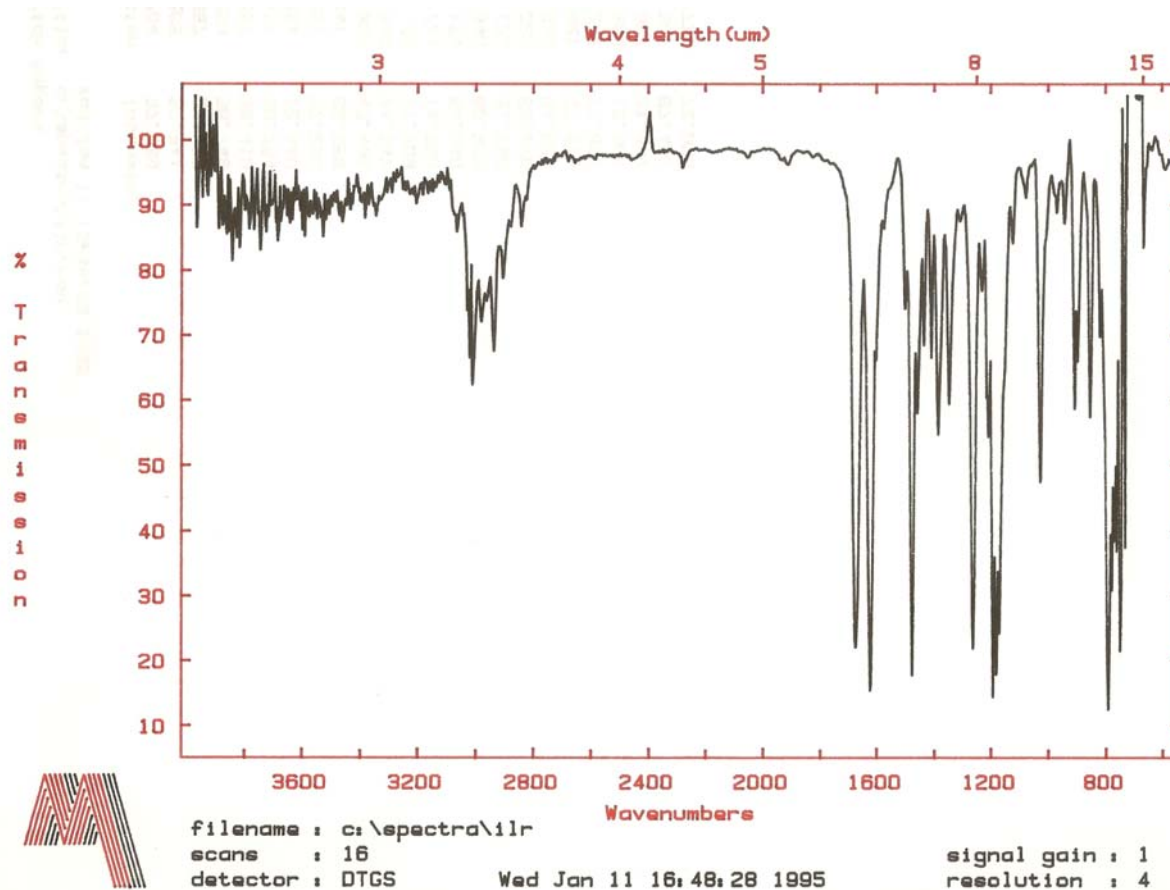


Problem R-08C (C₁₄H₁₄O₂)
 300 MHz ¹H NMR Spectrum in CDCl₃
 Source: Aldrich Spectra Collection/Reich g



IR Spectrum



Problem R-08C. You are given the 300 MHz ^1H NMR spectrum of a disubstituted naphthalene.

(a) Identify the two substituents, and summarize the NMR evidence that leads to that conclusion.

(b) What does the leaning of the peaks between δ 7.7 and 7.9 tell you?

(c) What does the leaning of the peaks between δ 7.1 and 7.25 tell you?

(d) For each of the 8 positions on the naphthalene as defined below, 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. You may assume that naphthalene NMR properties are similar to those of benzene.

1 _____

5 _____

2 _____

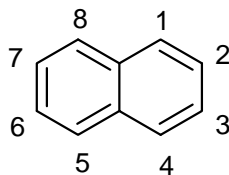
6 _____

3 _____

7 _____

4 _____

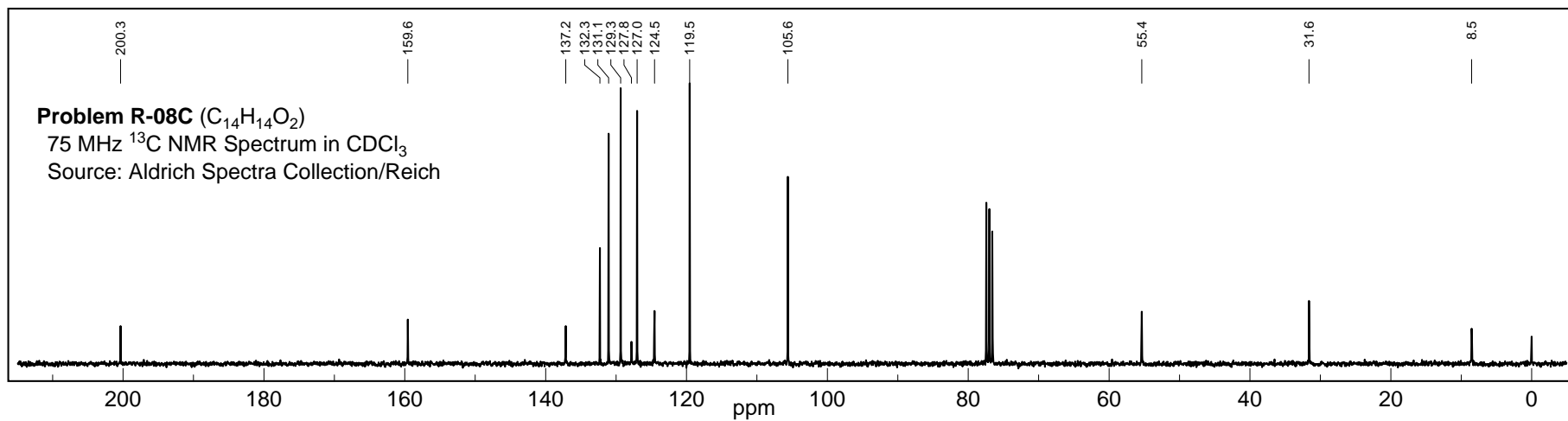
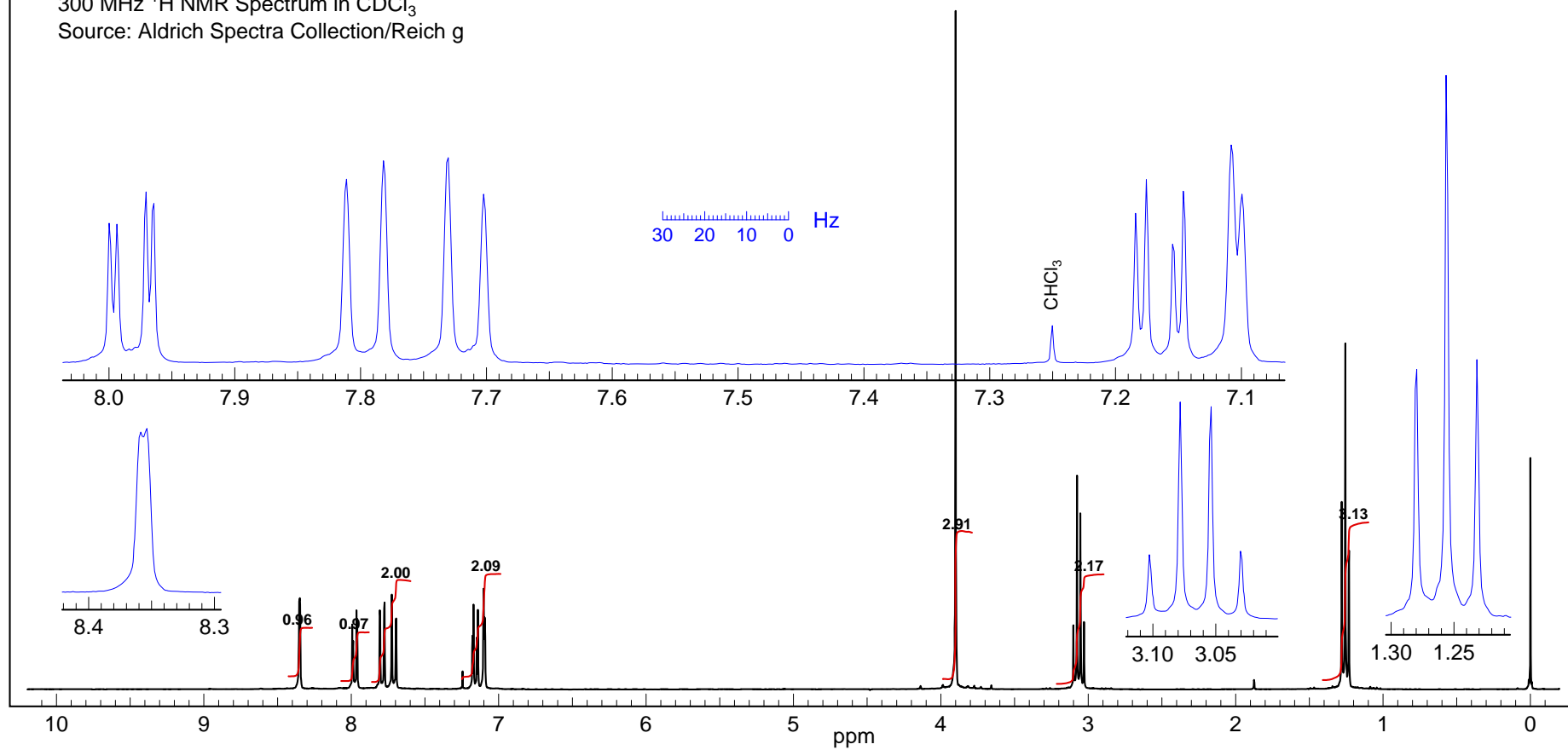
8 _____



Problem R-08C ($C_{14}H_{14}O_2$)

300 MHz 1H NMR Spectrum in $CDCl_3$

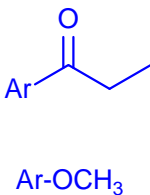
Source: Aldrich Spectra Collection/Reich g



18 Problem R-08C. You are given the 300 MHz ^1H NMR spectrum of a disubstituted naphthalene.

(a) Identify the two substituents, and summarize the NMR evidence that leads to that conclusion.

5



Ar-C(=O)CH₂CH₃
Ar-OCH₃

^{13}C - Carbonyl peak at δ 200.3, CH₃ at 8.5, CH₂ at 31.6 (propiophenone: 8.3, 31.7)
 ^1H - Me triplet at δ 1.26, CH₂ quartet at 3.07 (propiophenone: δ 1.17, 2.96)

^{13}C - CH₃O at δ 55.4 (Ph-OMe: δ 54.8)
 ^1H - Me singlet at δ 3.9 (Ph-OMe: δ 3.73)

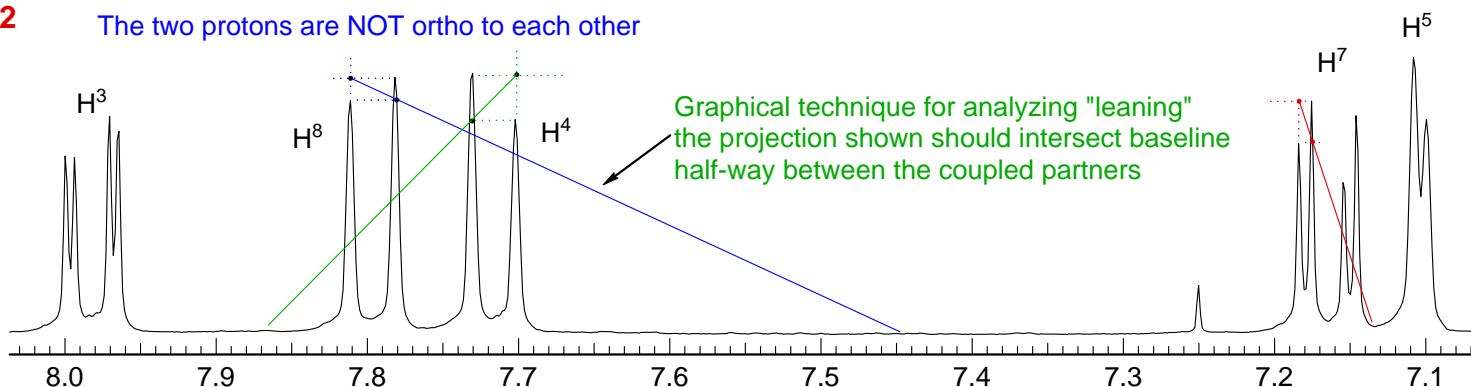
-Et
-CO₂Me

-CO₂Et
-Me

-OEt
-C(=O)Me

(b) What does the leaning of the peaks between δ 7.7 and 7.9 tell you?

These two doublets are not NOT coupled to each other - the leaning is much too small
 The one at 7.72 must be coupled to the one at 7.98, the one at 7.80 to the one at 7.16
2 The two protons are NOT ortho to each other



(c) What does the leaning of the peaks between δ 7.1 and 7.25 tell you?

2 These two protons are coupled to each other with a small coupling constant (ca 2 Hz, - meta coupling). They are meta to each other on the same ring, one of them is ortho-coupled to a distant proton

(d) For each of the 8 positions on the naphthalene as defined below, 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. You may assume that naphthalene NMR properties are similar to those of benzene.

1 8.36, d, J=1.5 Hz

5 7.10, d, J = 2

2 C(=O)CH₂CH₃

6 OMe

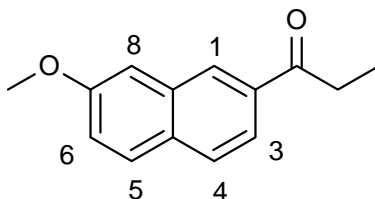
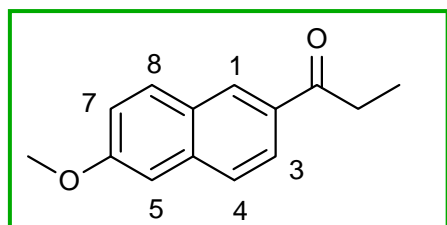
6 3 7.98, dd, J = 6, 1.5

7 7.16, dd, J = 8, 2 Hz

4 7.72, d, J = 6 Hz

8 7.80, d, J = 8 Hz

3



Hard to distinguish these