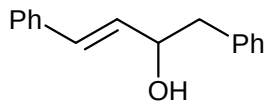
Problem R-87E ($C_{16}H_{16}O$)

270 MHz ^{1}H NMR spectrum in $CDCl_3$

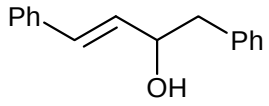
Source: J. W Ringer/Reich 11/17 (digitized hard copy) g



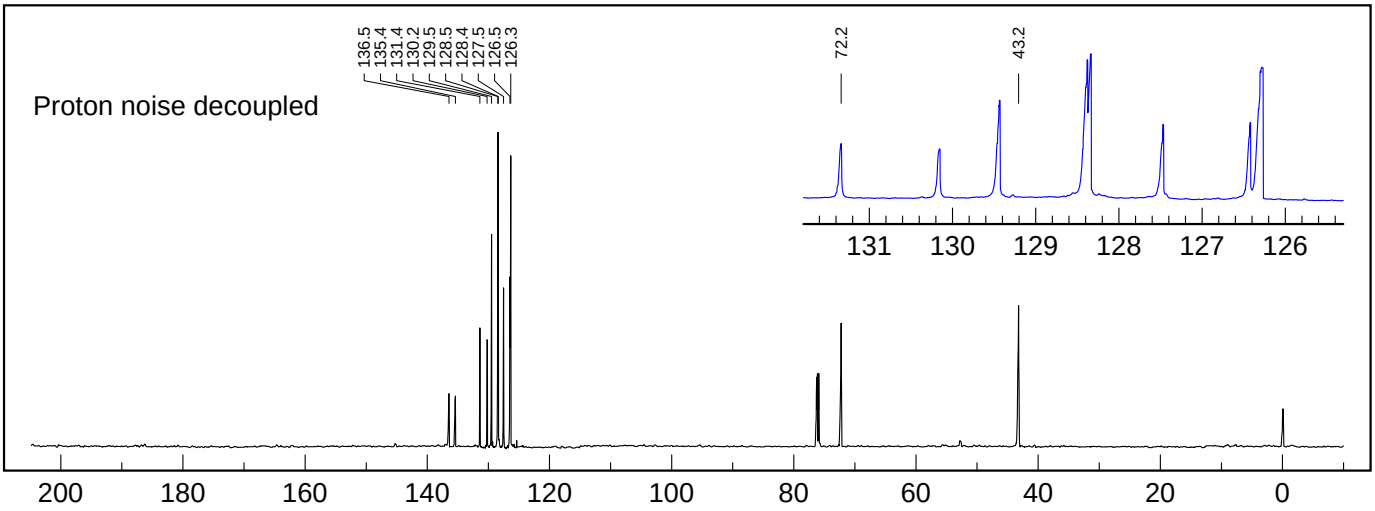
PLT pr-087-to-94.plt

Problem R-87E ($C_{16}H_{16}O$)
125 MHz ^{13}C NMR Spectrum in $CDCl_3$
(Source: J. W. Ringer/Reich 11/17)

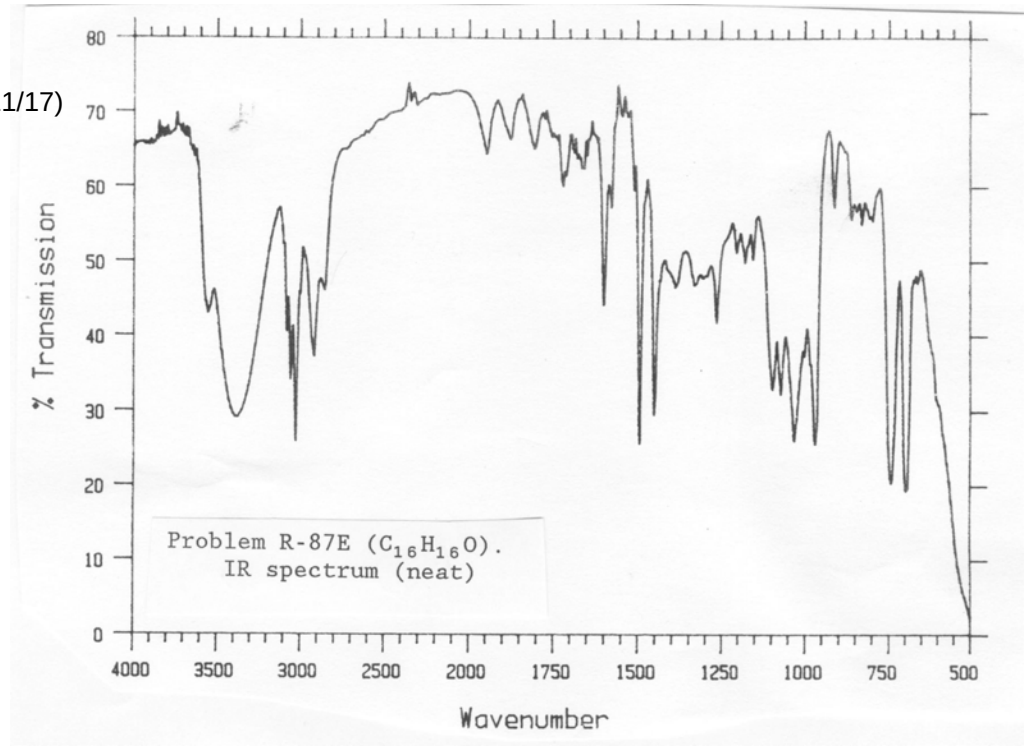
Fully coupled



Proton noise decoupled



Problem R-87E ($C_{16}H_{16}O$)
IR Spectrum neat
(Source: J. W. Ringer/Reich 11/17)



Problem R-87E. ($C_{16}H_{16}O$). The compound contains two phenyl groups (C_6H_5)

(a) DBE__

(b) Analyze the IR spectrum.

(c) Analyze each region of the proton NMR spectrum, draw part structures. Draw a possible structure for the compound and label protons with chemical shifts and coupling constants. Use the format: δ 1.23, dq, J = 9, 7 Hz.

1-2 δ

3 δ

4-5 δ

6-7 δ

7-8 δ

(d) Interpret key signals in the ^{13}C NMR spectra. The top spectrum is coupled, the bottom is noise proton decoupled. Do not attempt to make a detailed assignment to the signals between δ 125 and δ 135. The expansion provided is for your information only

(e) Draw the structure of the compound.

Problem R-87E. ($C_{16}H_{16}O$). The compound contains two phenyl groups (C_6H_5)

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(a) DBE 9 2 phenyls (8 DBE), one double bond (1 DBE)

(b) Analyze the IR spectrum.

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3400 cm^{-1}: OH H-bonded
3600 cm^{-1}: free OH
1600-1800 cm^{-1} - no strong peaks, so no C=O

(c) Analyze each region of the proton NMR spectrum, draw part structures. Draw a possible structure for the compound and label protons with chemical shifts and coupling constants. Use the format: δ 1.23, dq, J = 9, 7 Hz.

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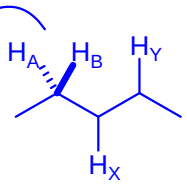
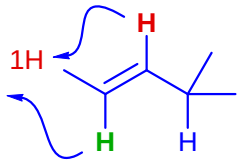
1-2 δ δ 1.8, 1H, broad singlet, probably an OH

3 δ AB of ABX(Y) pattern, 2H, δ_A = 3.03, δ_B = 2.94
J_{AB} = 14.7 Hz
J_{AX} = 5.6 Hz
J_{BX} = 8.5 HZ



4-5 δ X part of ABX, with additional coupling, sort of a ddd

6-7 δ δ 6.32, dd. *J* = 17.0, 6.8 Hz, 1H
δ 6.65, d. *J* = 17.0 Hz, 1H



7-8 δ 10H aromatic region - probably two phenyl groups

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(d) Interpret key signals in the ^{13}C NMR spectra. The top spectrum is coupled, the bottom is noise proton decoupled. Do not attempt to make a detailed assignment to the signals between δ 125 and δ 135. The expansion provided is for your information only

δ 73.4, d

δ 44.1, t

δ 130-140 10 sp^2 carbons

Since there are 12 carbon signals. and the molecule has 16C, there must be 4 doubled carbons. These are the ortho and meta carbons of the two phenyls, nicely seen in the expansion. The 10 sp^2 signals must be 8 aromatic C, and 2 double bond C.

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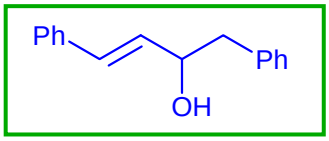
(e) Draw the structure of the compound.



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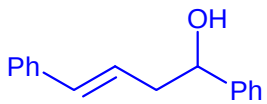
Other structures proposed:



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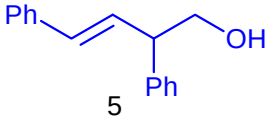

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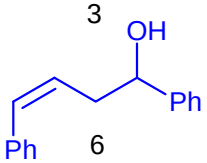

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