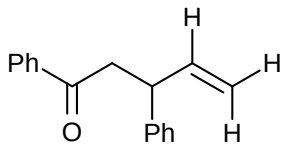
Problem R-08J ($C_{17}H_{16}O$)

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

Source: Art Cammers/Ed Vedejs (Reich digitized hard copy) g



PLT ex-2-2008-09-gq.plt

Problem R-08J ($C_{17}H_{16}O$). This problem requires you to solve the structure of a compound from the ^{1}H NMR spectrum.

(a) DBE __ . (b) The IR spectrum has a strong peak at 1695 cm-1. What does this tell you about the compound?

(c) Analyze each of the signals in the NMR spectrum. If appropriate, report δ, J, multiplicity, and number of hydrogens (e.g., δ 1.3. dq, J = 7, 3 Hz, 1H). You may use first order analysis. Give any part structure the signal identifies.

A _____

B _____

C _____

D _____

E _____

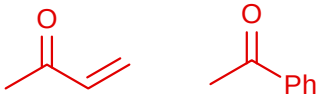
(d) Draw the structure of **R-08J**. Label the protons with the letters above (**A**, **B**, **C**, etc).

Problem R-08J ($C_{17}H_{16}O$). This problem requires you to solve the structure of a compound from the ^1H NMR spectrum.

2 (a) DBE 10. (b) The IR spectrum has a strong peak at 1695 cm-1. What does this tell you about the compound?

Since there is only one oxygen, this frequency corresponds well to a conjugated ketone

3



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A

δ 7.92, dm, J = 8 Hz, 2H
2 aromatic H ortho to carbonyl

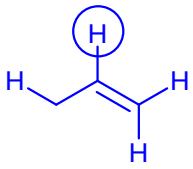
δ 7.2-7.7, 8H
Rest of aromatic H's

Together, likely two Ph groups, one with an electron withdrawing substituent

B

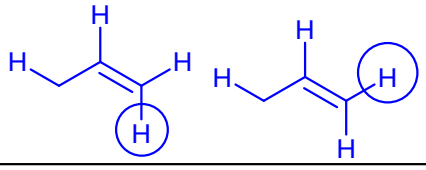
Vinyl proton, with $^3J_{cis}$, $^3J_{trans}$, and ^3J to a CH2

δ 6.06, ddd, J = 16.5. 9.5, 6 Hz, 1H



C

δ 5.04, dt, J = 16.5. 2 Hz, 1H
δ 5.06, dt, J = 10, 2 Hz, 1H

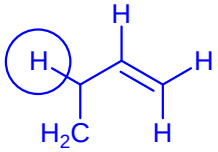


Common wrong answer is selecting 4/10 Hz couplings. Can rule out based on leaning.

14

D

δ 4.17, qm (app qt), J = 6 Hz, 1H
This is actually ddddd (five different couplings) but 3 are almost the same (^3J = 6 Hz) as are two others (^4J, too small to resolve)



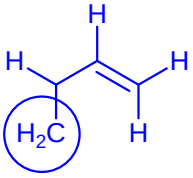
Since there are no methyl groups, must be a CH-CH-CH_2 type of apparent quartet

E

AB of ABX (δ 3.44, dd, J = 16.5, 6 Hz, 1H)

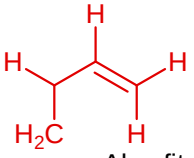
AB of ABX (δ 3.37, dd, J = 16.5, 6 Hz, 1H)

Must be an asymmetric center



(d) Draw the structure of **R-08J**. Label the protons with the letters above (**A**, **B**, **C**, etc).

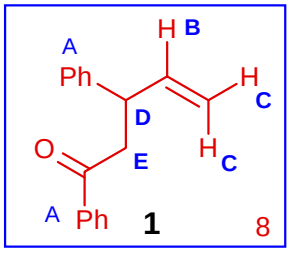
NMR gives



+ C(=O) + Ph + Ph

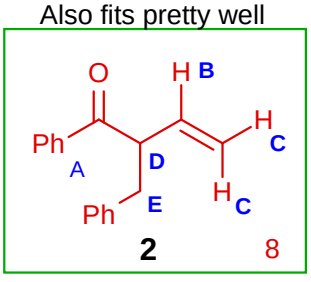
10

Actual Structure



D_{calc} = 3.45

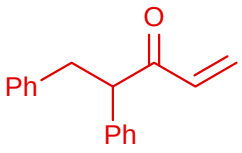
Also fits pretty well



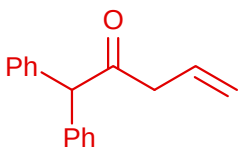
D_{calc} = 3.75

Obs:4.2

1 is the actual structure, but **2** fits well also, and even calculates better for the δ of H^D. ^2J for H^E fits better for **1**, as does the δ of H^A.

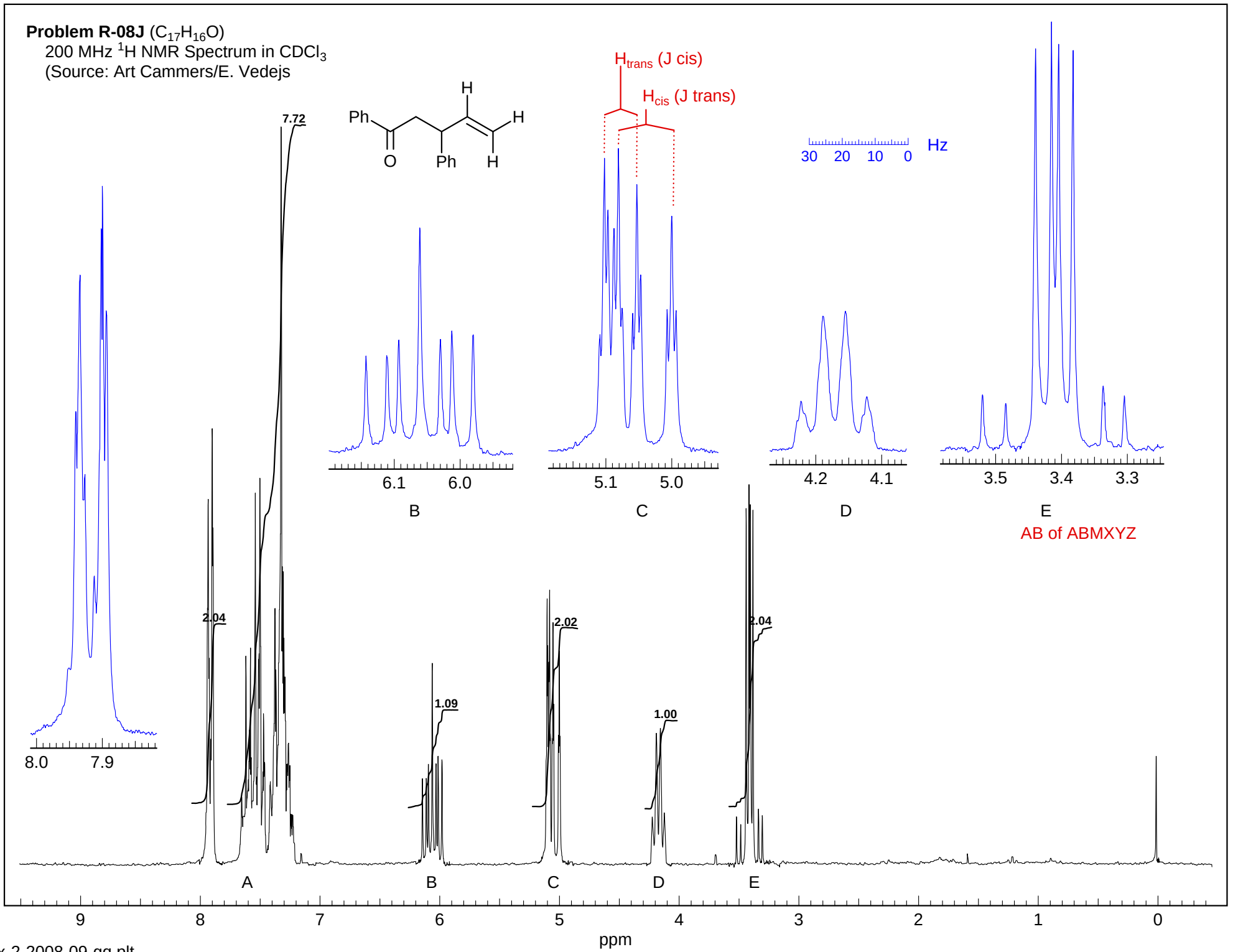


4



3

All other structures <3


Problem R-08J (C17H16O)
200 MHz 1H NMR Spectrum in CDCl3
(Source: Art Cammers/E. Vedejs
Ph
H
O
Ph
H
H
Htrans (J cis)
Hcis (J trans)
30 20 10 0
Hz
7.72
2.04
1.09
2.02
1.00
2.04
8.0 7.9
6.1 6.0
5.1 5.0
4.2 4.1
3.5 3.4 3.3
B
C
D
E
AB of ABMXYZ
A
B
C
D
E
9 8 7 6 5 4 3 2 1 0
ppm
PLT ex-2-2008-09-gq.plt