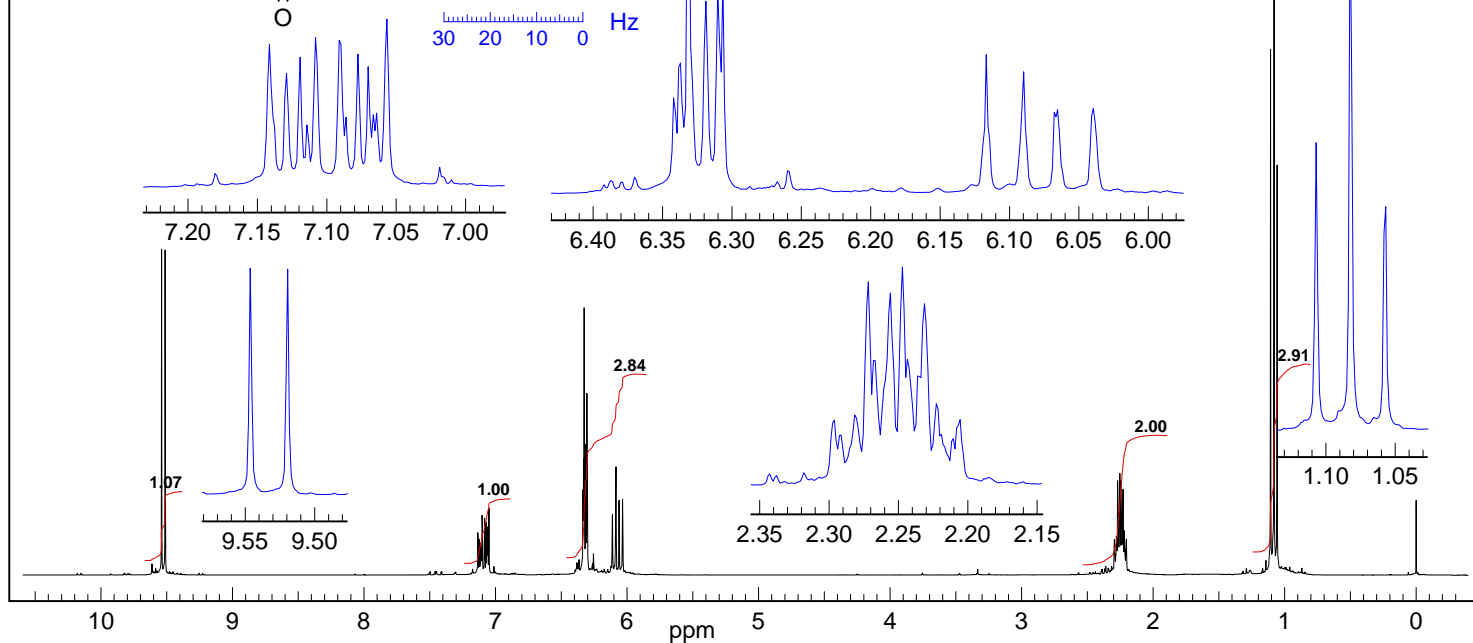
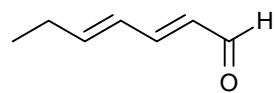
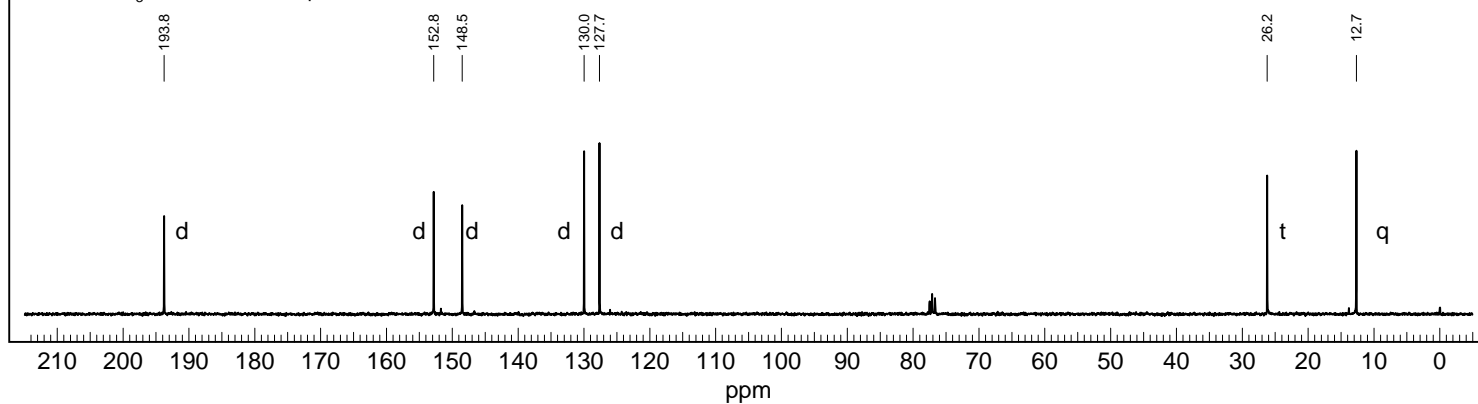
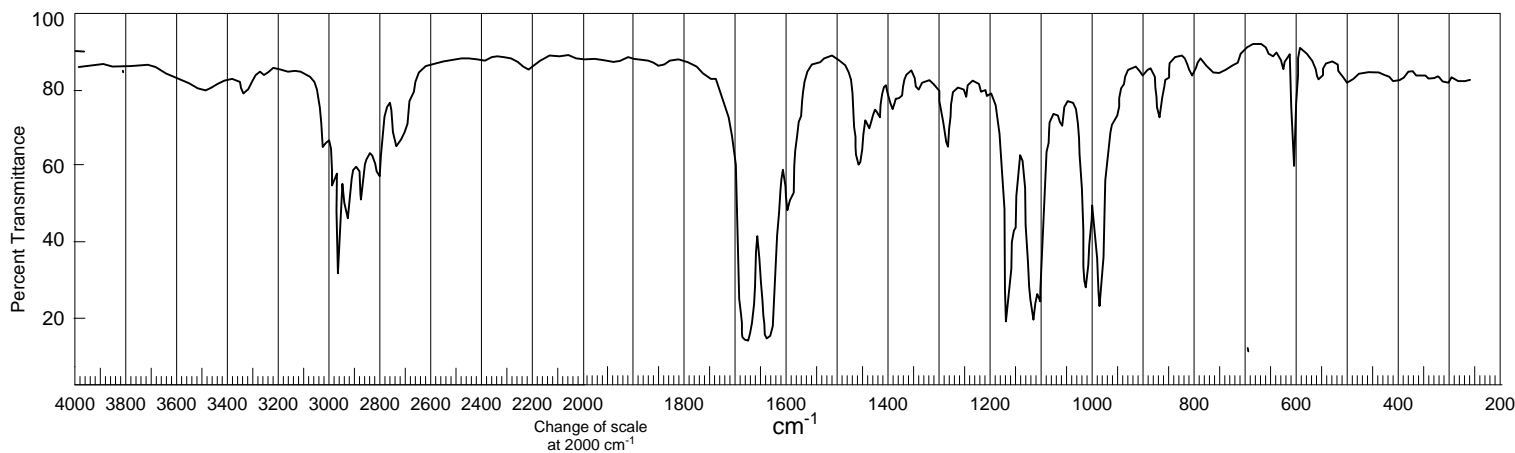


Problem R-85C ($C_7H_{10}O$)300 MHz 1H NMR spectrum in $CDCl_3$

Source: Aldrich Spectra Collection/Reich 33-09 g

**Problem R-85C:** $C_7H_{10}O$ 75 MHz ^{13}C NMR spectrumSolv: $CDCl_3$; Source: Aldrich Spectra Collection/Reich

Infrared Spectrum:



Problem R-85C ($C_7H_{10}O$). Determine the structure of the compound from the 1H and ^{13}C NMR spectra, and the IR spectrum.

(a) DBE? _____

(b) Define part structures or functional groups from examination of the various spectra. Briefly explain your reasoning.

(i) IR spectrum:

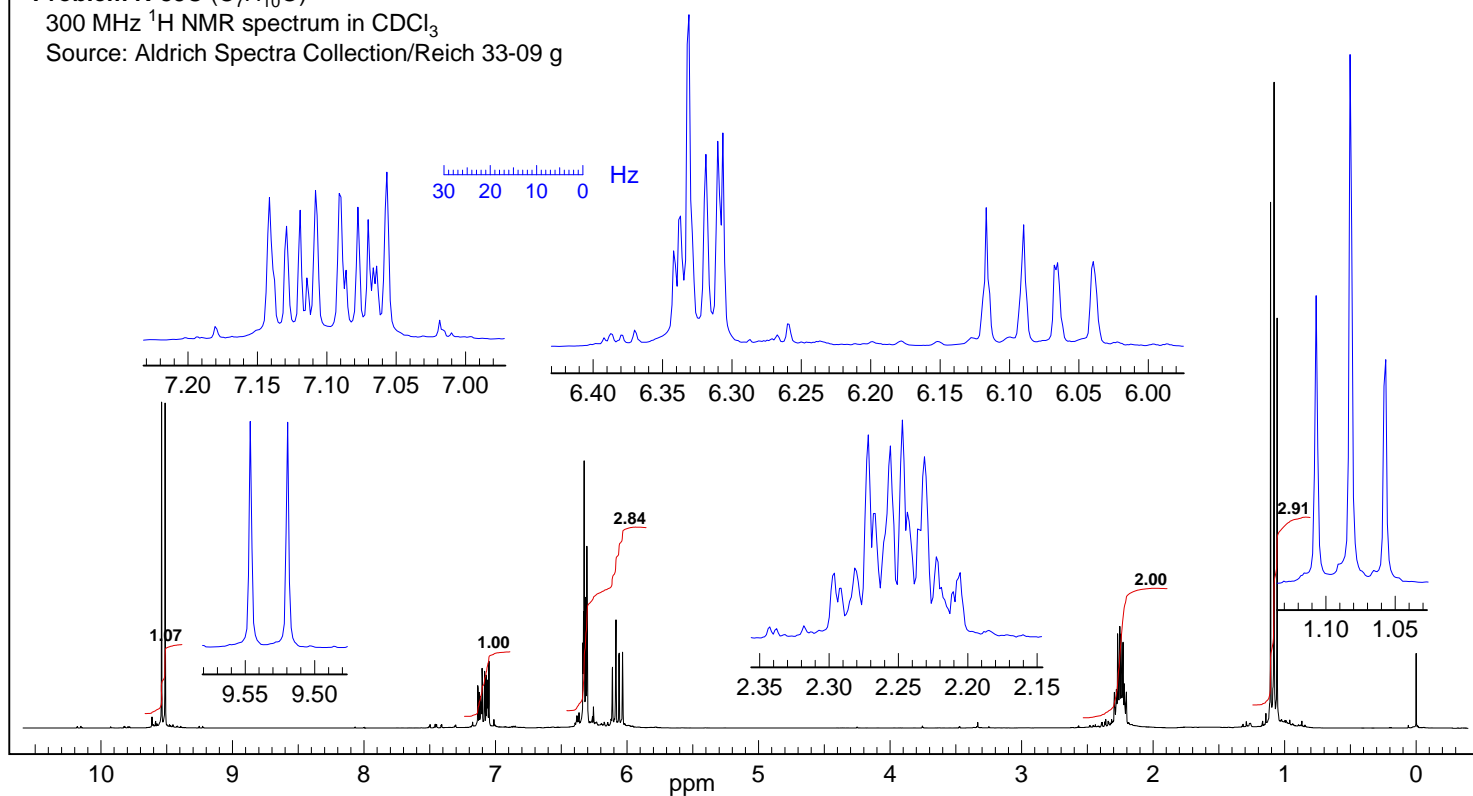
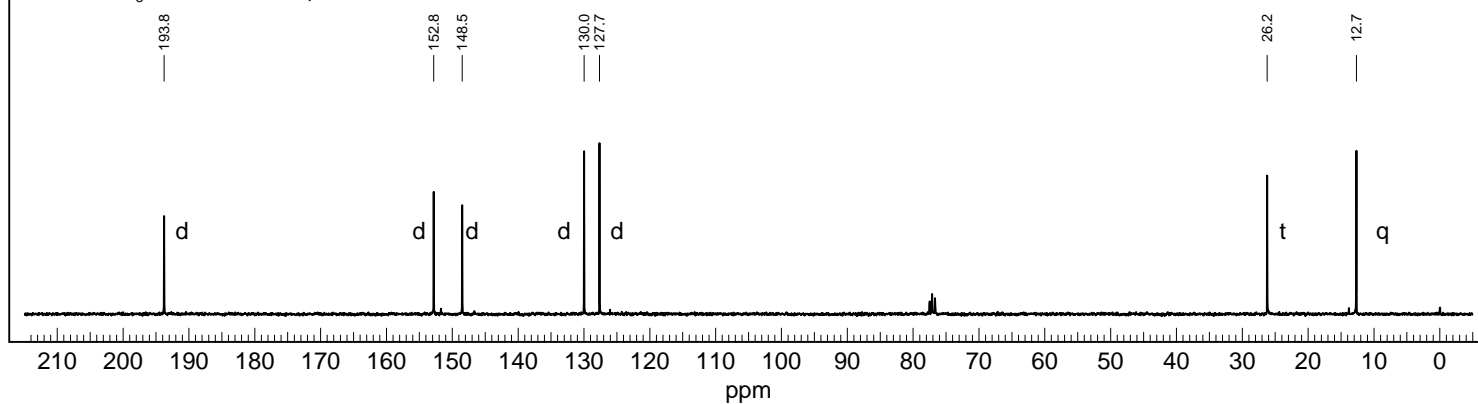
(ii) ^{13}C NMR spectrum:

(iii) 1H NMR spectrum

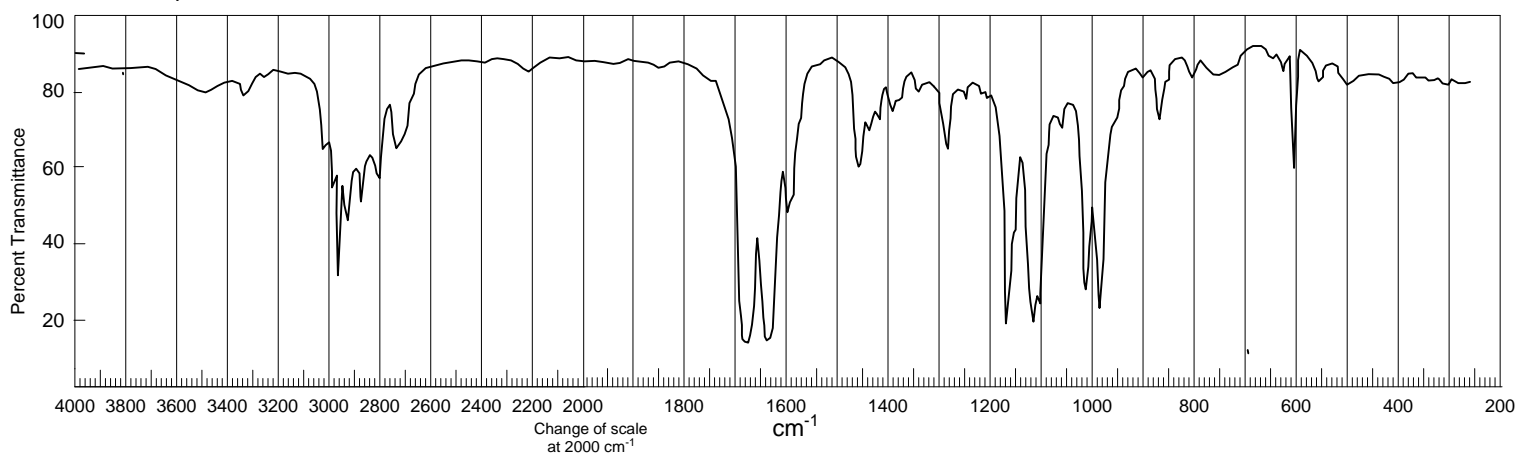
(c) Structure of **R-86C**.

Problem R-85C ($C_7H_{10}O$)300 MHz 1H NMR spectrum in $CDCl_3$

Source: Aldrich Spectra Collection/Reich 33-09 g

**Problem R-85C:** $C_7H_{10}O$ 75 MHz ^{13}C NMR spectrumSolv: $CDCl_3$; Source: Aldrich Spectra Collection/Reich

Infrared Spectrum:



Problem R-85C ($C_7H_{10}O$). Determine the structure of the compound from the 1H and ^{13}C NMR spectra, and the IR spectrum.

(a) DBE? 3

(b) Define part structures or functional groups from examination of the various spectra. Briefly explain your reasoning.

(i) IR spectrum:

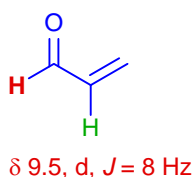
- Carbonyl at 1680 cm^{-1} , 1640 cm^{-1} - conjugated ketone/aldehyde, double bond
- 2830 cm^{-1} - CH stretch of aldehyde
- 960 cm^{-1} - CH bend of trans $HC=CH$
- no OH
- no 700 cm^{-1} for cis $HC=CH$

(ii) ^{13}C NMR spectrum:

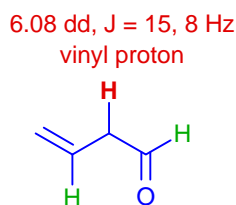
- $193.8\text{ H}-\overset{\text{O}}{\underset{\text{||}}{\text{C}}}$, probably conjugated (unconjugated are near 200 ppm)
- two peaks at 150, two at 130: probably two double bonds $HC=CH$, likely conjugated from downfield shift
- 12.7 (CH_3) 26.2 (CH_2). ^{13}C NMR does not tell us they are connected (as in CH_2-CH_3), but 1H does.

This accounts for all carbons, hydrogens and the oxygen

(iii) 1H NMR spectrum

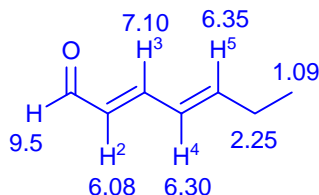


1.09 (t, $J = 7$)
 CH_3-CH_2-CH
 2.25 approximate dq,
 $J = 7, 5\text{ Hz}$



Multiplets at 6.32 and 7.10 are 3 more vinyl protons, with a lot of second order coupling

(c) Structure of **R-86C**



The first double bond stereochemistry is well defined as *trans* by the 15 Hz coupling of the dd at $\delta\ 6.08$ (H^2). The other double bond is not so simple to define from the NMR spectra (the IR gives a hint), but probably also *trans*, from the large AB-coupling in the multiplet at $\delta\ 6.32$. These are H^4 and H^5 , which form an **ABMX2** pattern with J_{AB} ca 15 Hz. A at ca $\delta\ 6.35$ is coupled to the CH_2 , B at ca 6.30 coupled the neighboring $HC=$. It requires computer simulation to define this with more confidence.

The multiplets at 2.25 (H^6) and 7.10 (H^3) show second order effects because they are coupled to the close-coupled protons at 6.32 (H^4 and H^5)