

CHEM202

Organic Chemistry

Nick Green

nick.green@otago.ac.nz, 3n11

Module 1: Spectroscopy and Characterisation

Lecture 6: Interpreting ^1H NMR Spectra

NMR has been associated with 6 Nobel
Prizes

- Obtaining data from spectra.
- Structural Elucidation

^1H NMR Analysis

Apply the mnemonic NIPS (For simple first order systems)

N = No. of sets of signals

gives the number of different kinds of protons in the compound.

I = Integration

gives the number of protons of each kind by using the integrated area.

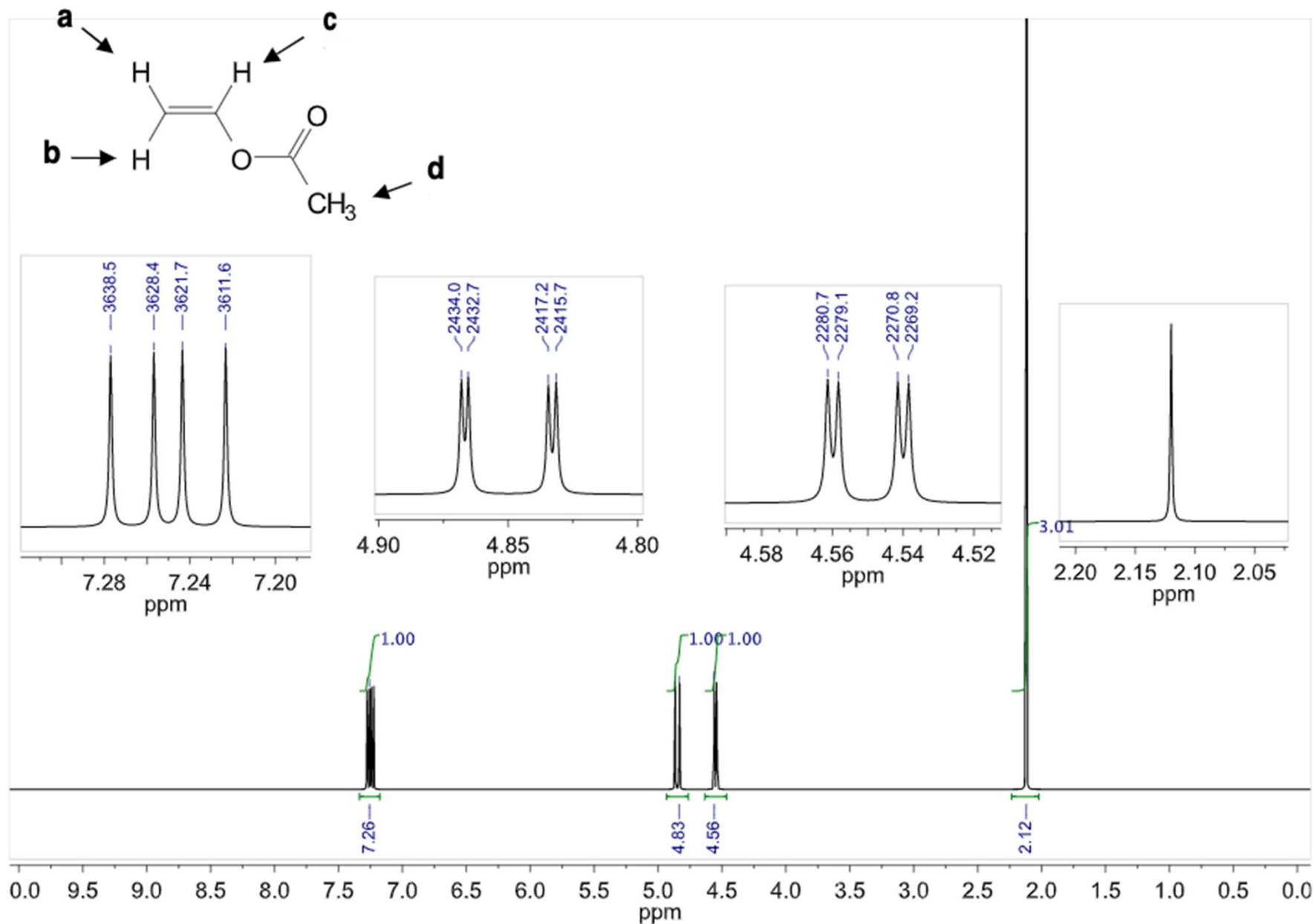
P = Position

δ value gives information about the environment.
Tables of chemical shift values are available for comparison

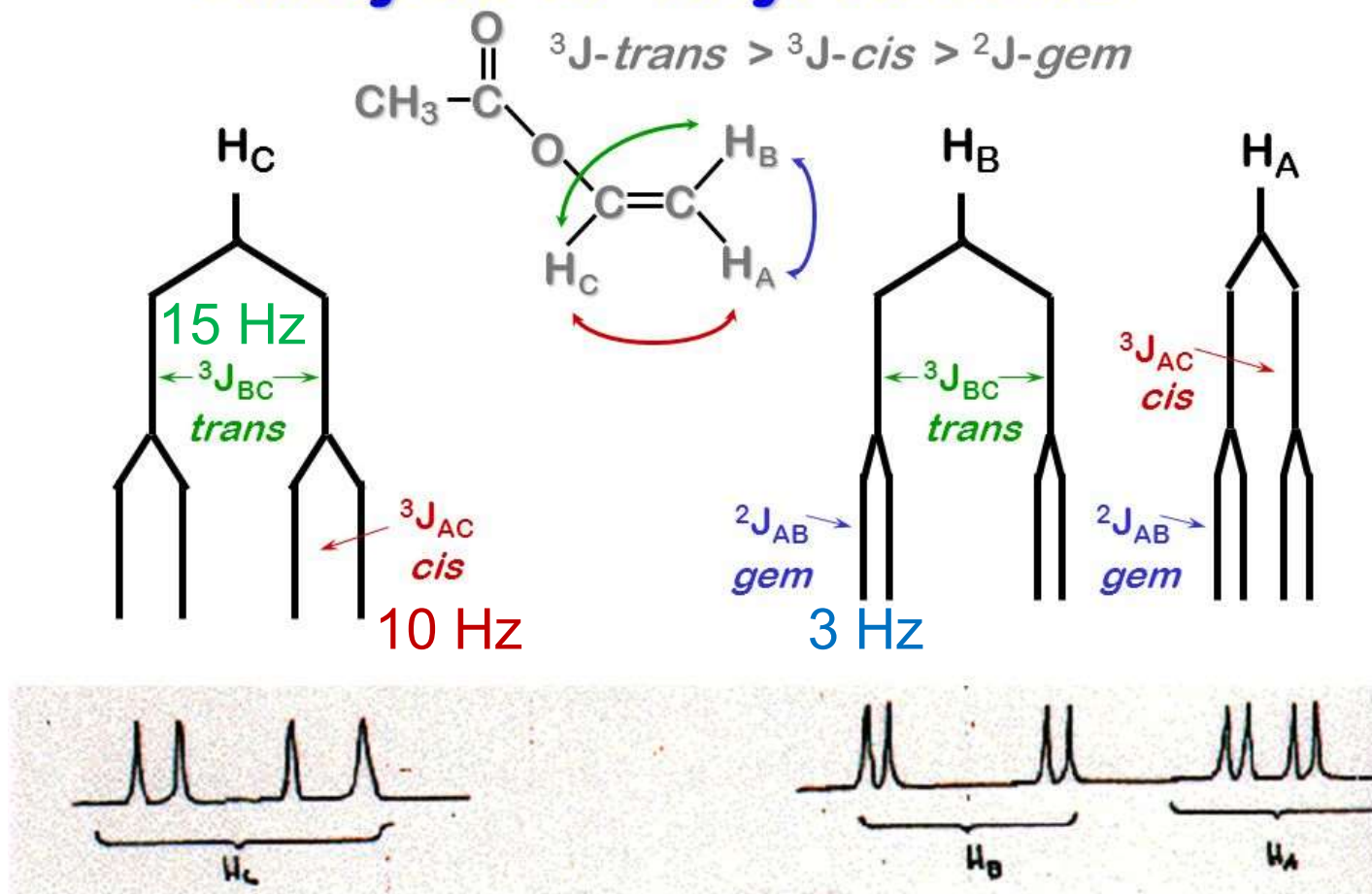
S = Splitting Pattern

gives information about the number of protons on the adjacent C atoms.

^1H NMR of vinyl acetate

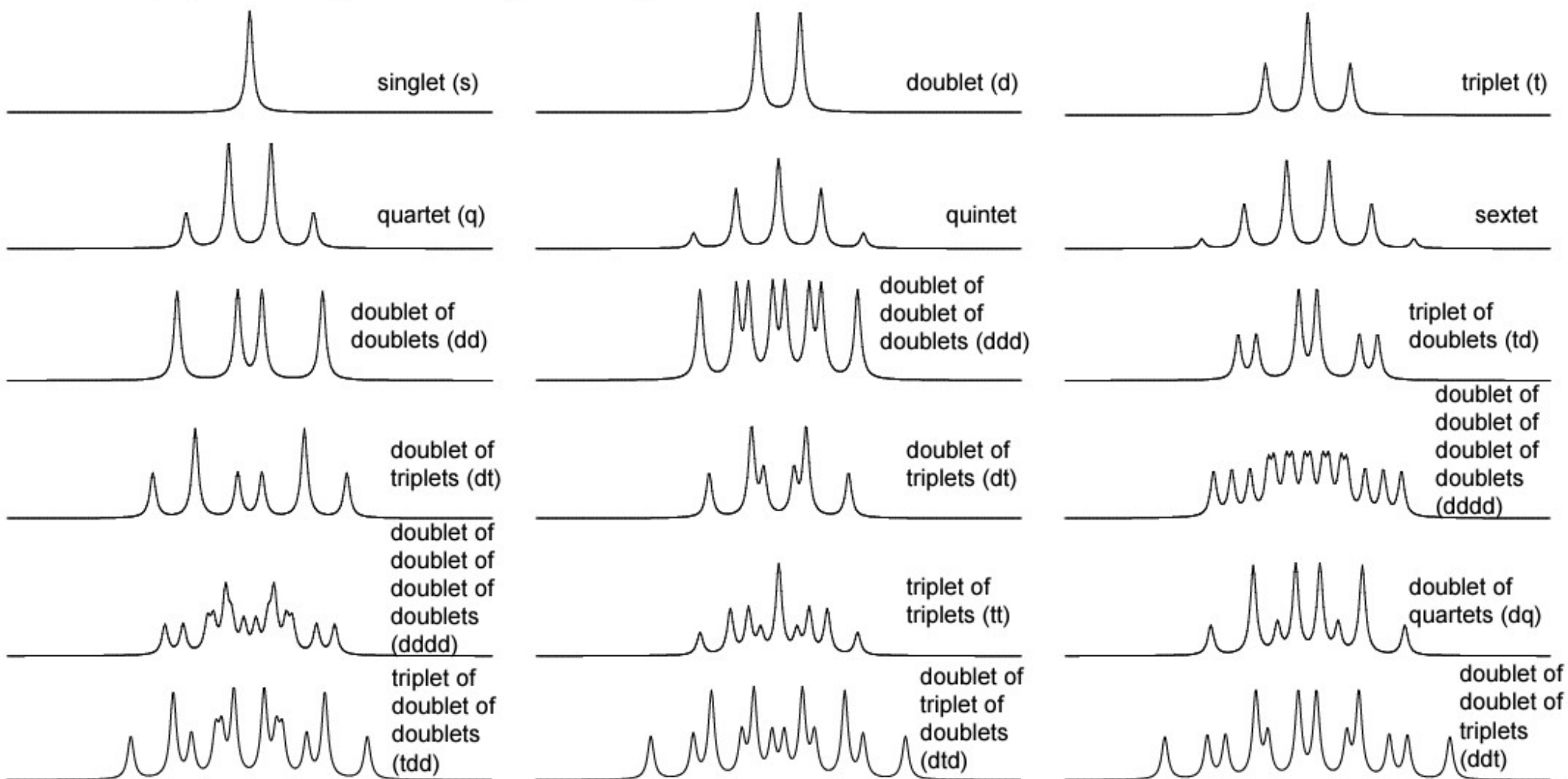


Analysis of Vinyl Acetate

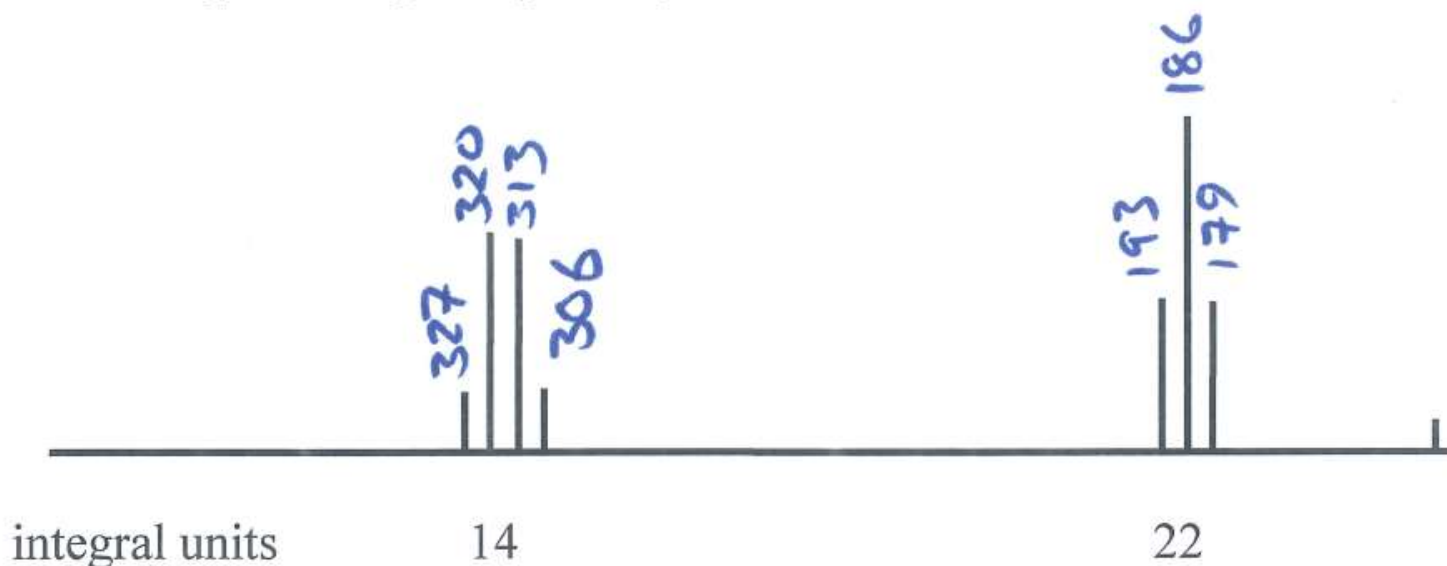


Each signal is a doublet of doublets (dd)
i.e. the signal is split into a doublet twice, with a corresponding coupling constant J (splitting gap) for each split

Splitting by multiple non equivalent neighbours

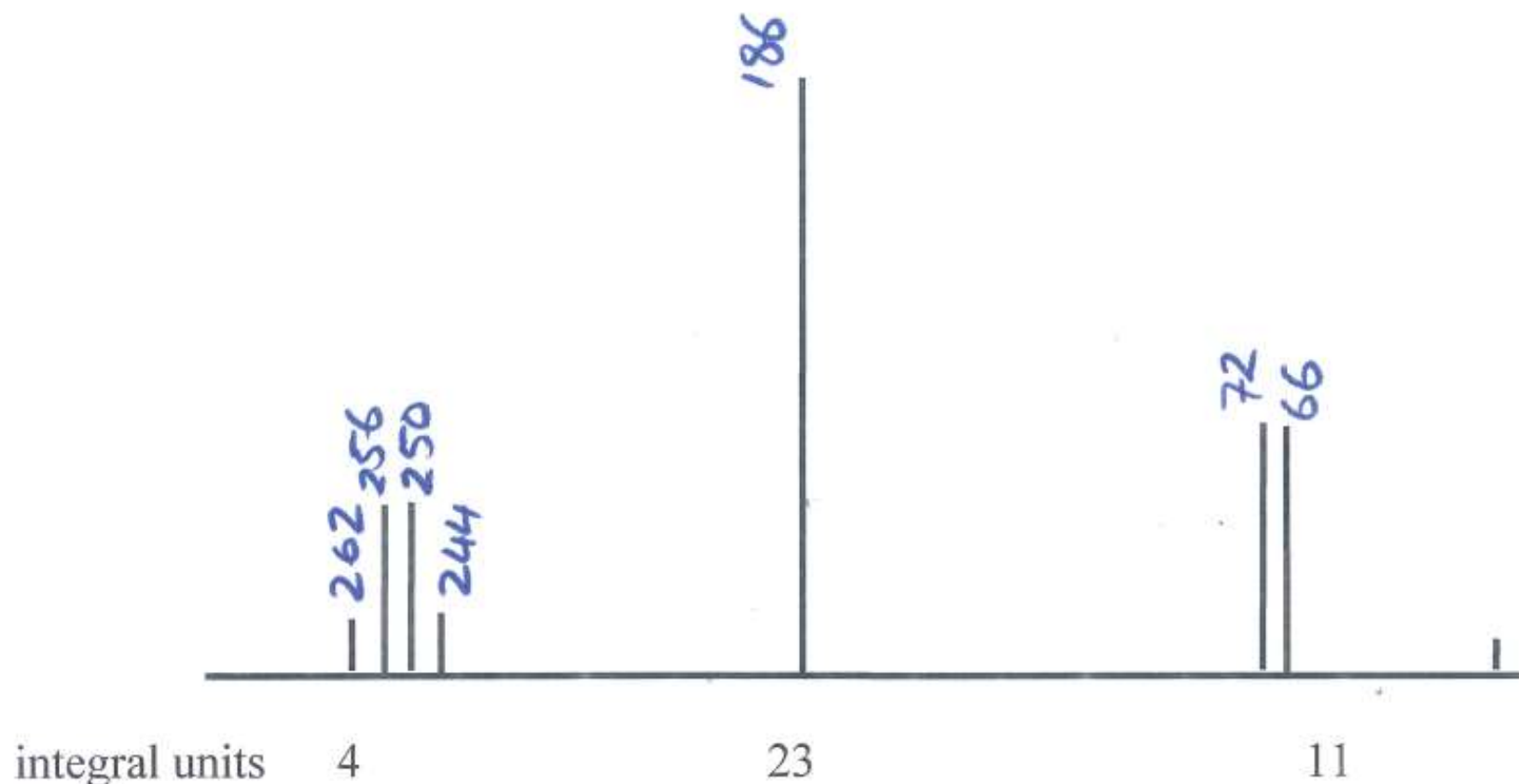


^1H nmr of ethyl iodide obtained on a spectrometer with an operating frequency of 100 MHz

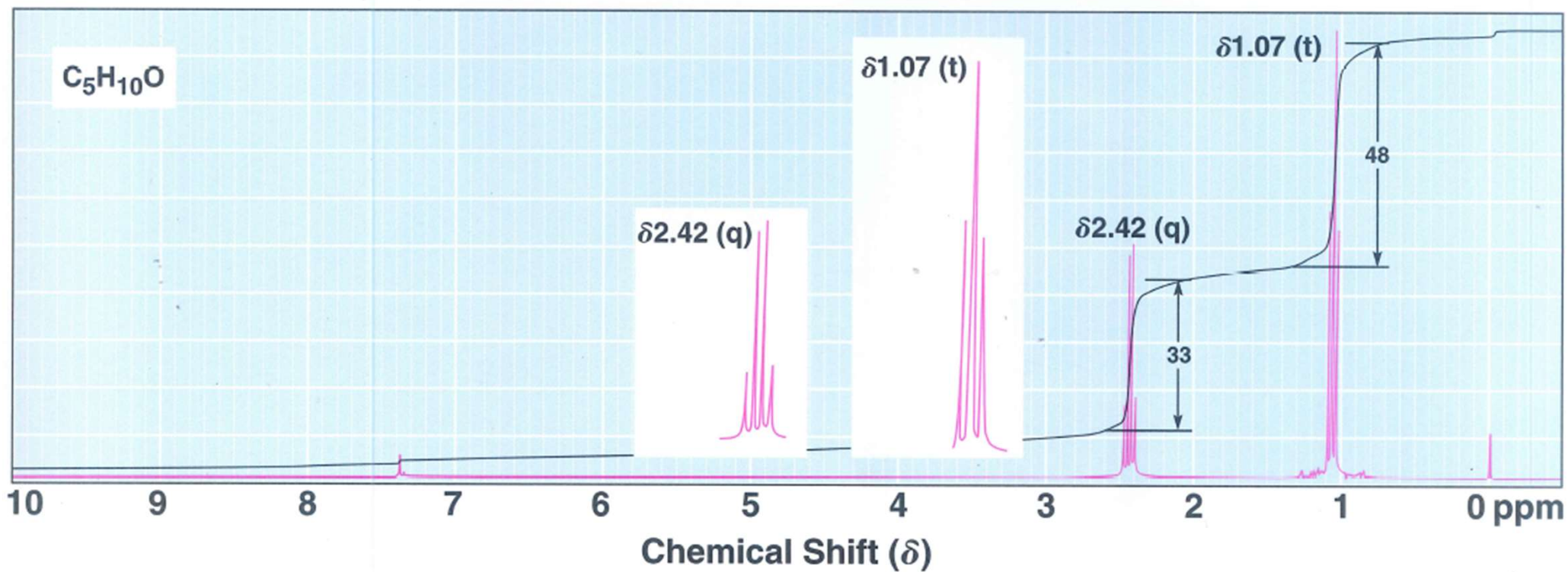


- Calculate the δ and J values for the observed signals.
- Tabulate the data
- Calculate the line frequencies of the spectrum when measured at 300 MHz.

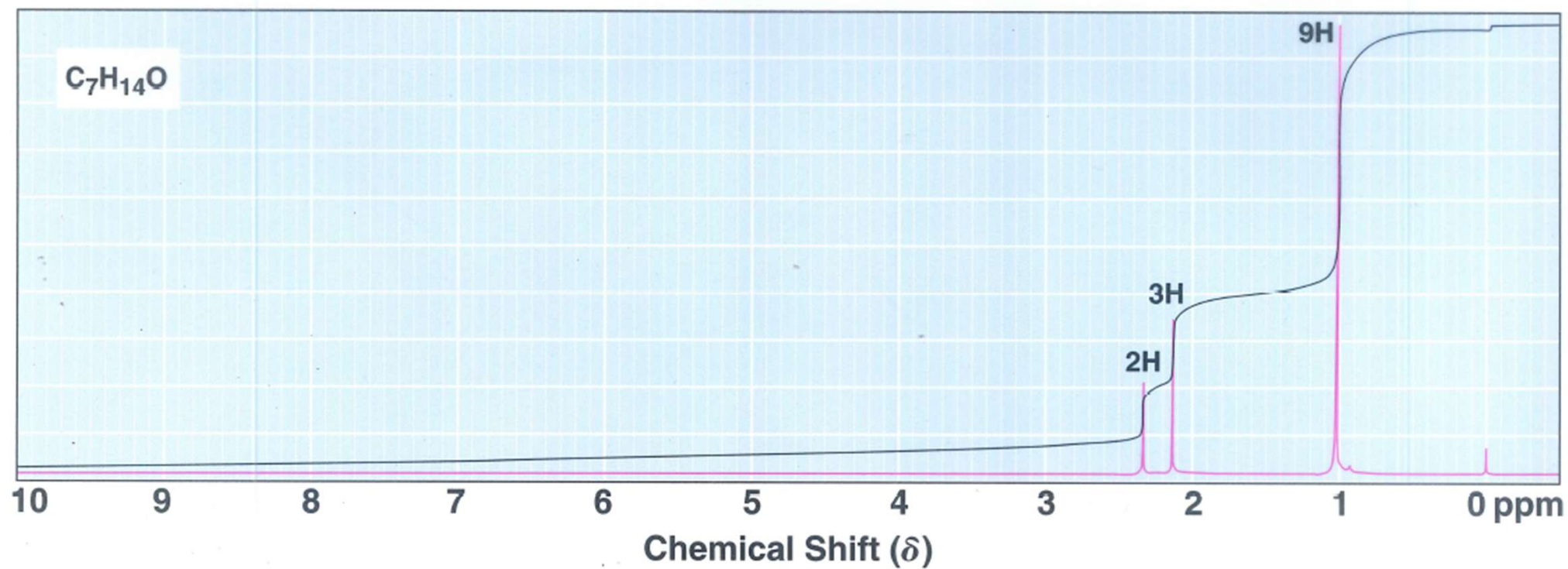
- Tabulate the ^1H nmr data, obtained on a spectrometer with an operating frequency of 60 MHz, for $\text{C}_4\text{H}_{10}\text{O}_2$.
- Deduce a possible structure for the compound.



^1H NMR of $\text{C}_5\text{H}_{10}\text{O}$



^1H NMR of $\text{C}_7\text{H}_{14}\text{O}$



Online Resources

Blackboard

Lectures/ Module 1: Structural Characterisation and Analysis

[Organic Chemistry Online: - Spectroscopy](#)

[Structure elucidation problem sets \(Notre Dame\)](#)