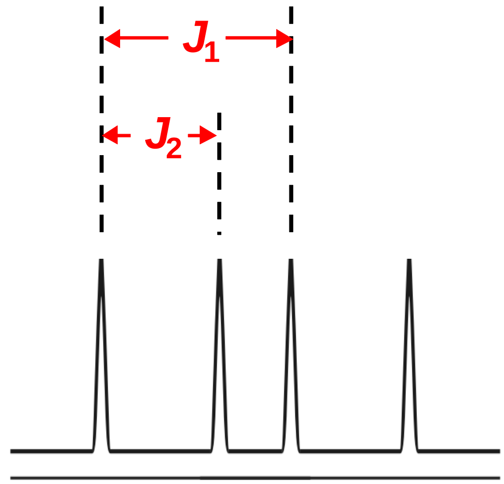
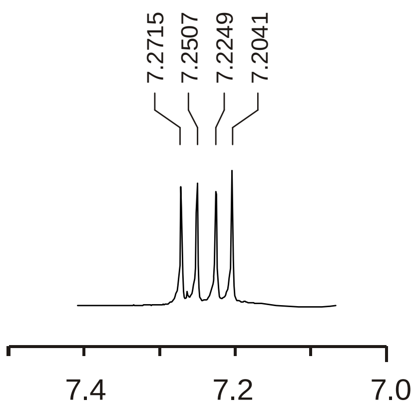
Workshop 29 Solutions
Complex Splitting Patterns in NMR

When we covered complex splitting patterns in lecture, I showed the simplest complex splitting pattern (if you will), the doublet of doublets; I also showed that the two coupling constants J_1 and J_2 that give rise to this pattern can be calculated by measuring the distance between peaks 1 and 2 (for J_1) and between peaks 1 and 3 (for J_2). There are three such patterns in this spectrum, corresponding to the three protons on the left-hand side of the molecule.

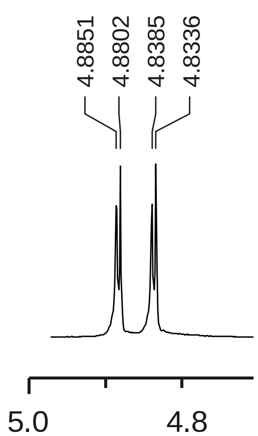


a. So, for each of those multiplets,



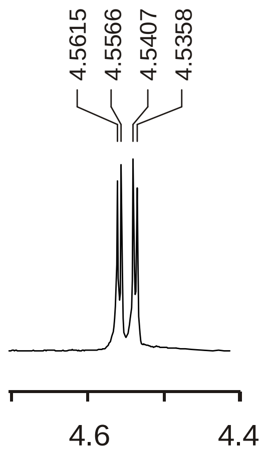
J_1: $\Delta\delta$ = (7.2715 ppm) – (7.2249 ppm)
= 0.0466 ppm
J_1 (Hz) = (0.0466 ppm) × (300 MHz)
= 14.0 Hz

J_2: $\Delta\delta$ = (7.2715 ppm) – (7.2507 ppm)
= 0.0208 ppm
J_1 (Hz) = (0.0208 ppm) × (300 MHz)
= 6.2 Hz



J_1: $\Delta\delta$ = (4.8851 ppm) – (4.8385 ppm)
= 0.0466 ppm
J_1 (Hz) = (0.0466 ppm) × (300 MHz)
= 14.0 Hz

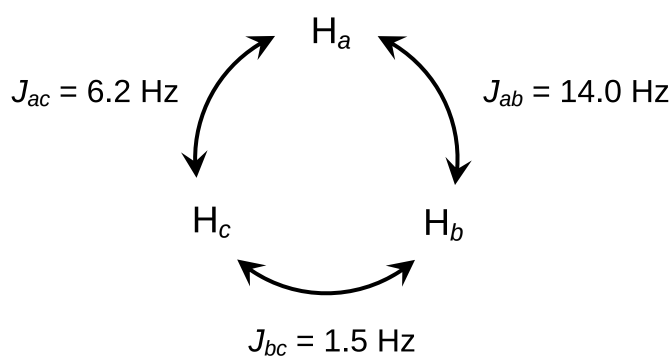
J_2: $\Delta\delta$ = (4.8851 ppm) – (4.8802 ppm)
= 0.0049 ppm
J_1 (Hz) = (0.0049 ppm) × (300 MHz)
= 1.5 Hz



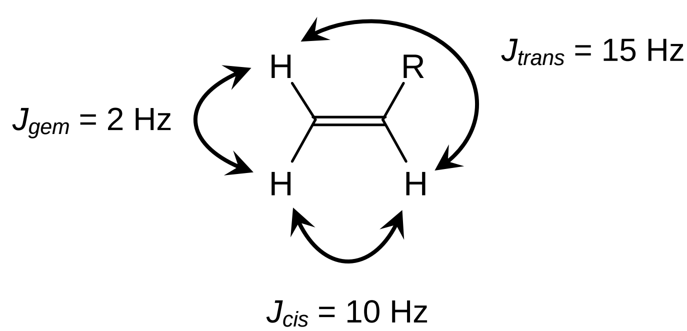
J_1: $\Delta\delta$ = (4.5615 ppm) – (4.5407 ppm)
= 0.0208 ppm
J_1 (Hz) = (0.0208 ppm) × (300 MHz)
= 6.2 Hz

J_2: $\Delta\delta$ = (4.5615 ppm) – (4.5566 ppm)
= 0.0049 ppm
J_1 (Hz) = (0.0208 ppm) × (300 MHz)
= 1.5 Hz

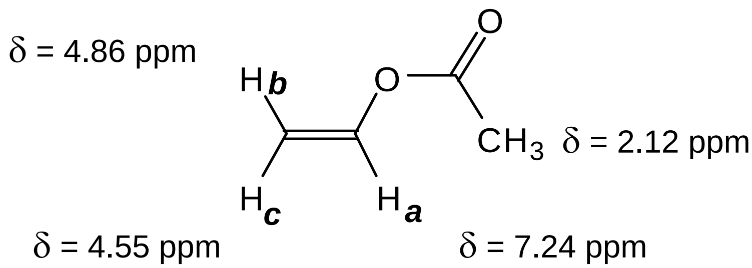
Importantly, each of the coupling constants in each multiplet matches one in another multiplet. That's because coupling constants between two nuclei are the same in both directions. So that means the three peaks represent three protons coupled to each other like



b. So then which proton in vinyl acetate is which? The chart of J values I showed in class says that typically,



These values are pretty close to the ones measured in the multiplets. (Yes, 6.2 Hz is quite a bit less than 10 Hz, but the trend is there.) So, the full NMR assignment would be:



J_{ab} = 14.0 Hz
J_{bc} = 1.5 Hz
J_{ac} = 6.2 Hz