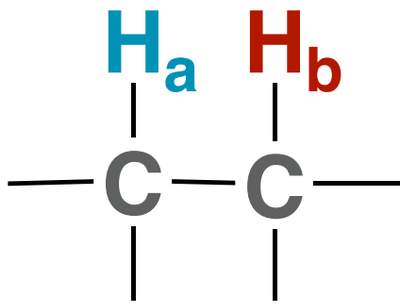
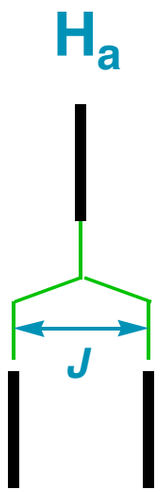
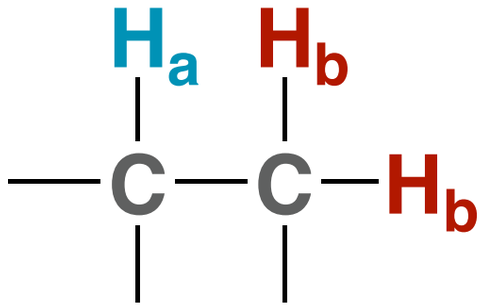
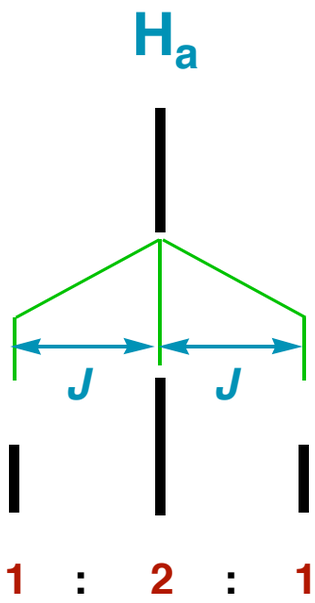
From Last Lecture

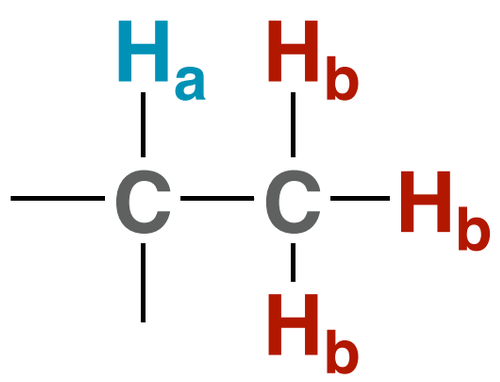
- Area under the peaks corresponds to relative number of hydrogens
- Resonances will split into n+1 peaks.

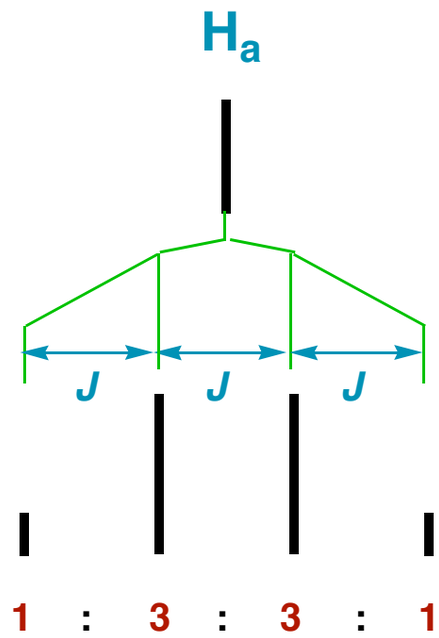










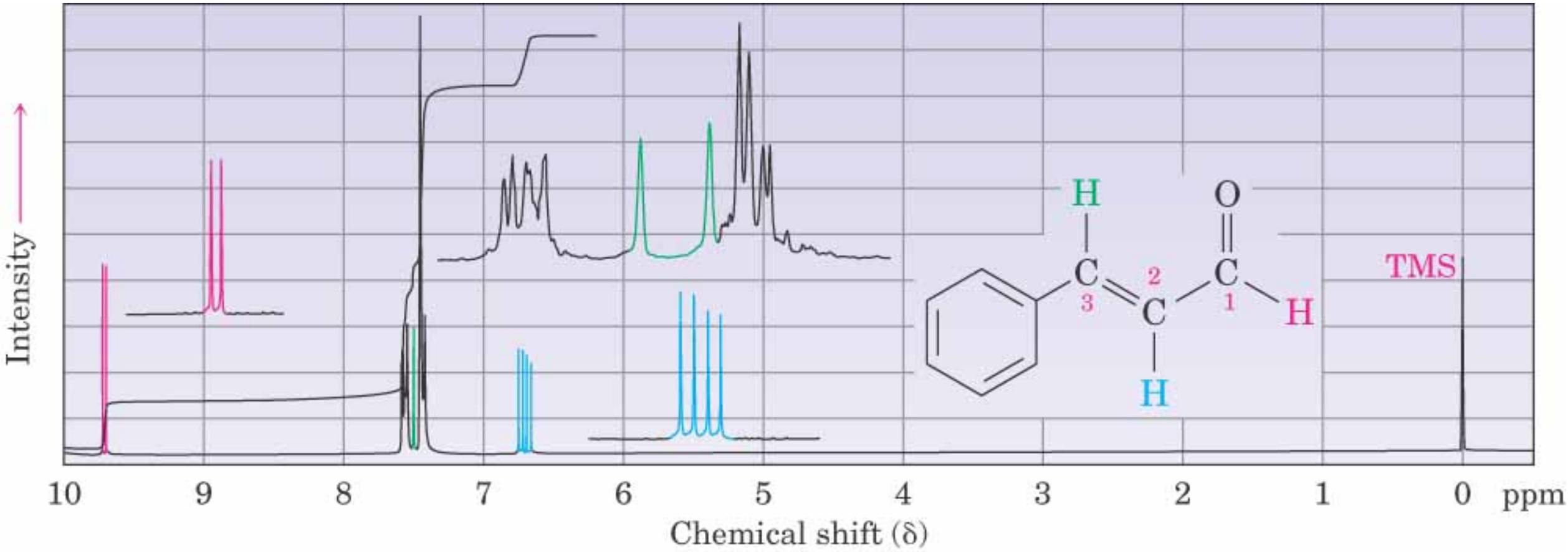


From Last Lecture

- Relative ratio of peaks depends on number of spin states of the neighbors (Pascal's Triangle)
- Adjacent protons will couple with the same coupling constant.
- Protons farther away usually do not couple.
- Chemically equivalent protons cannot couple (eg. $ClCH_2CH_2Cl$).

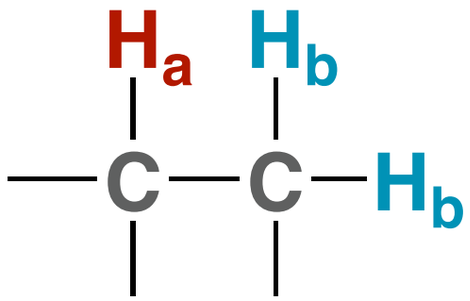
Cinnamaldehyde

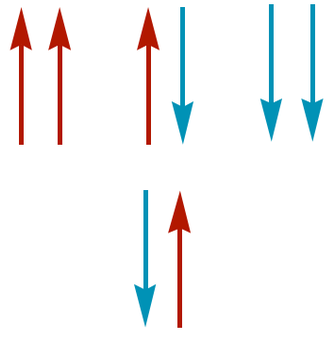
Multiple Coupling



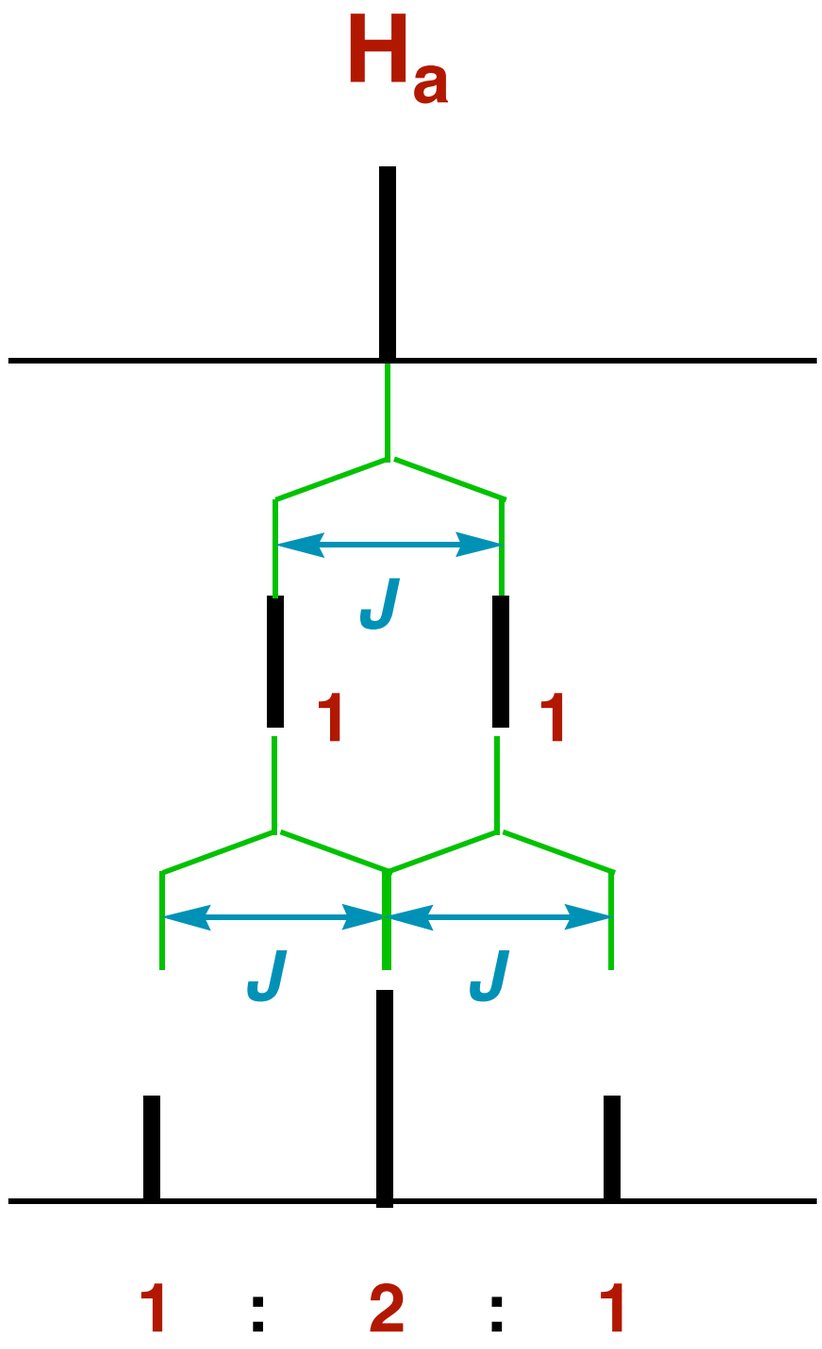
Spin Spin Splitting

- Every splitting can be broken down into a series of doublets





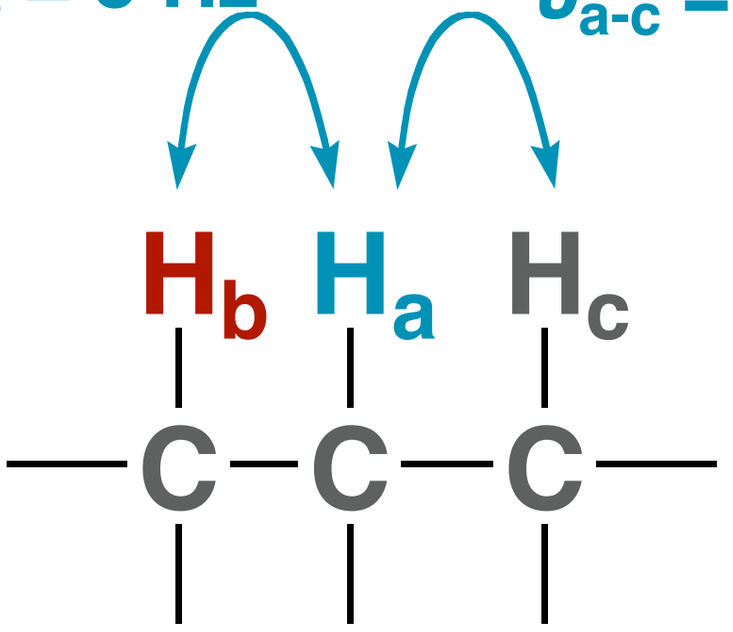
^{1}H NMR (without coupling)

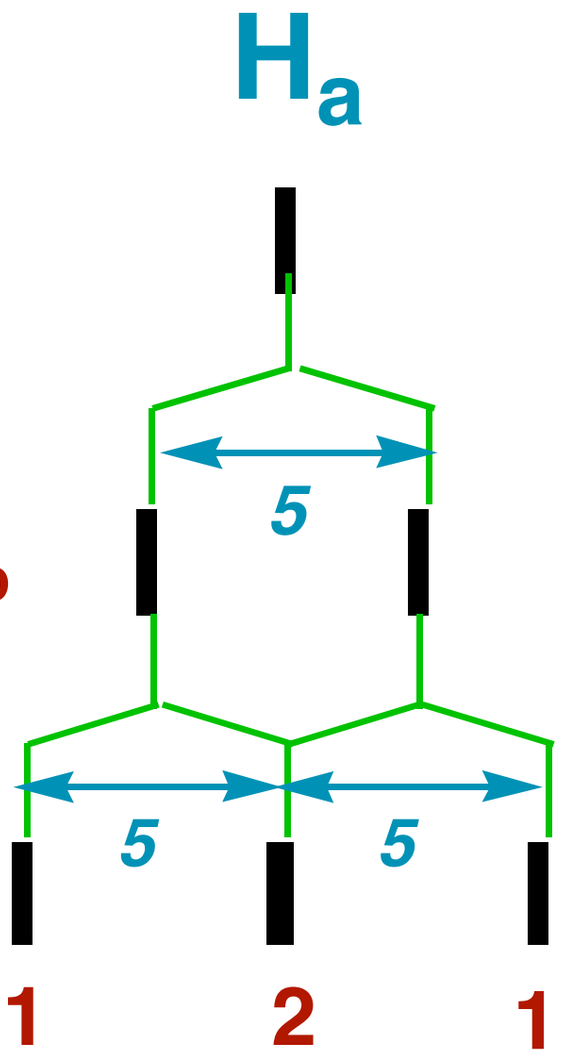


^{1}H NMR (with coupling)

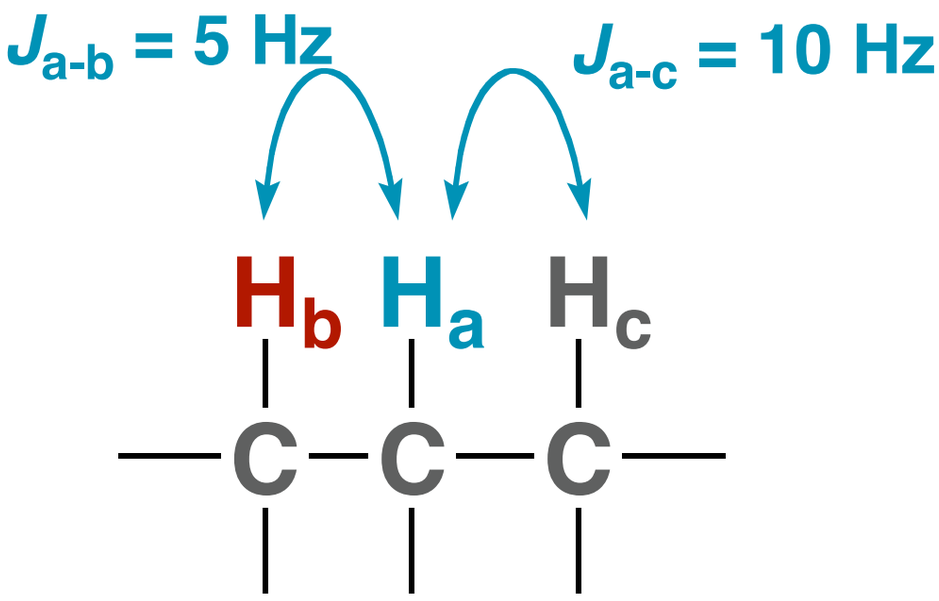
Coupling with the same *J*

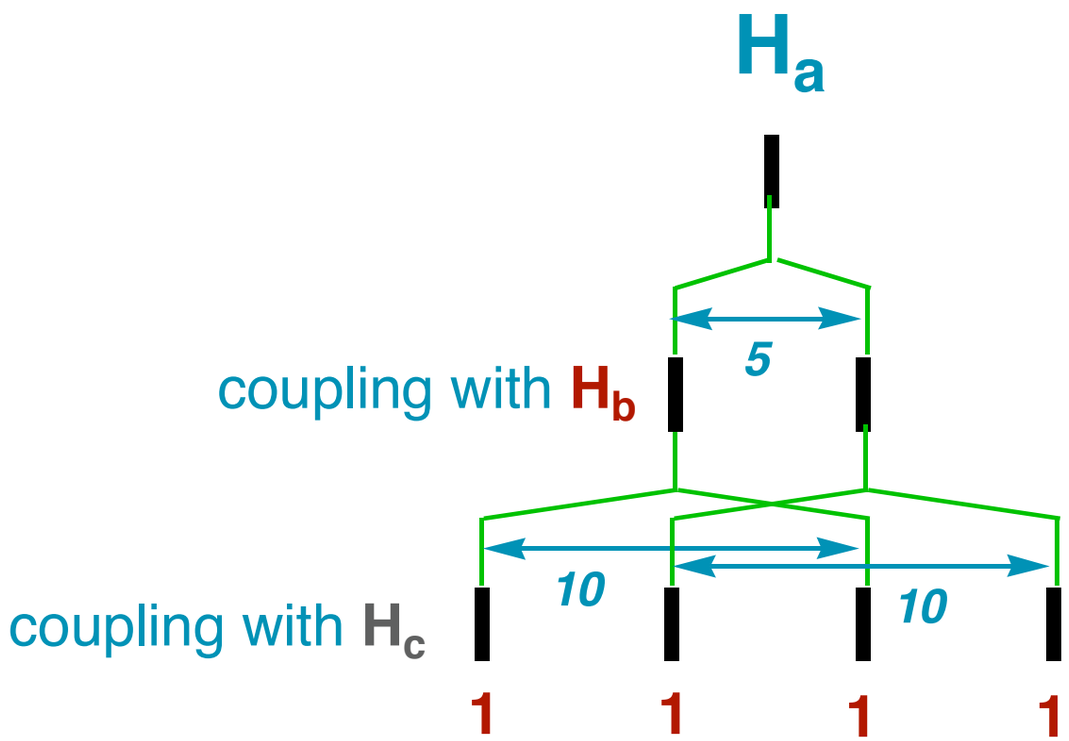
$J_{a\text{-}b}$ = 5 Hz $J_{a\text{-}c}$ = 5 Hz

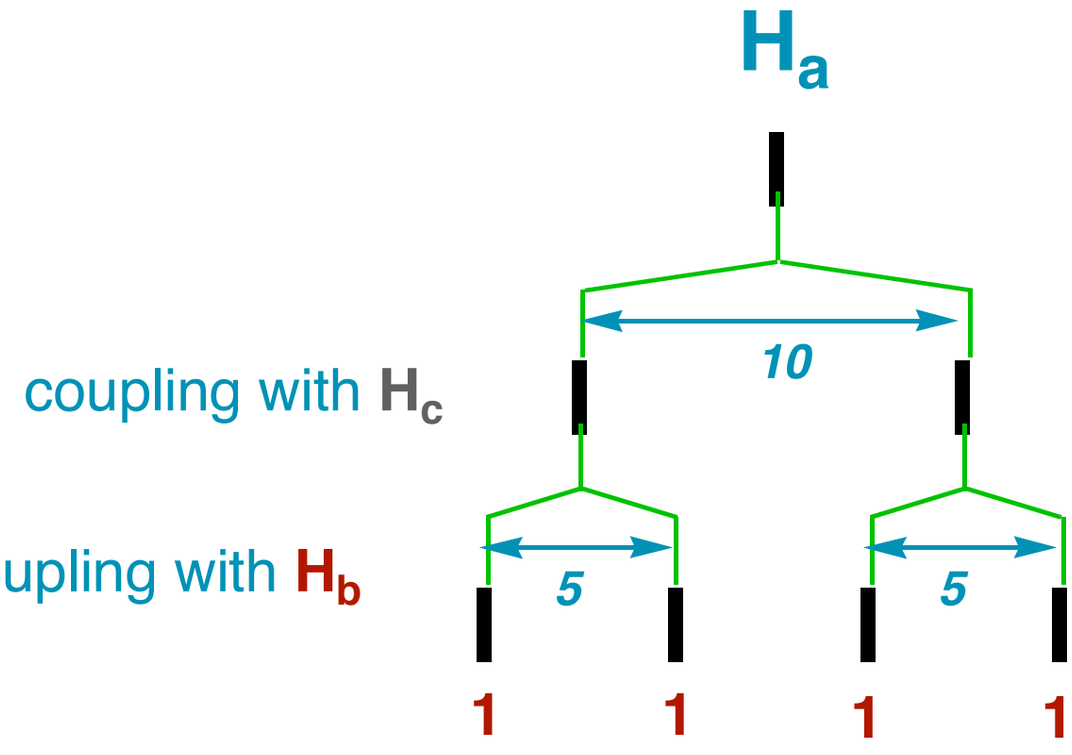




Coupling with different *J* values

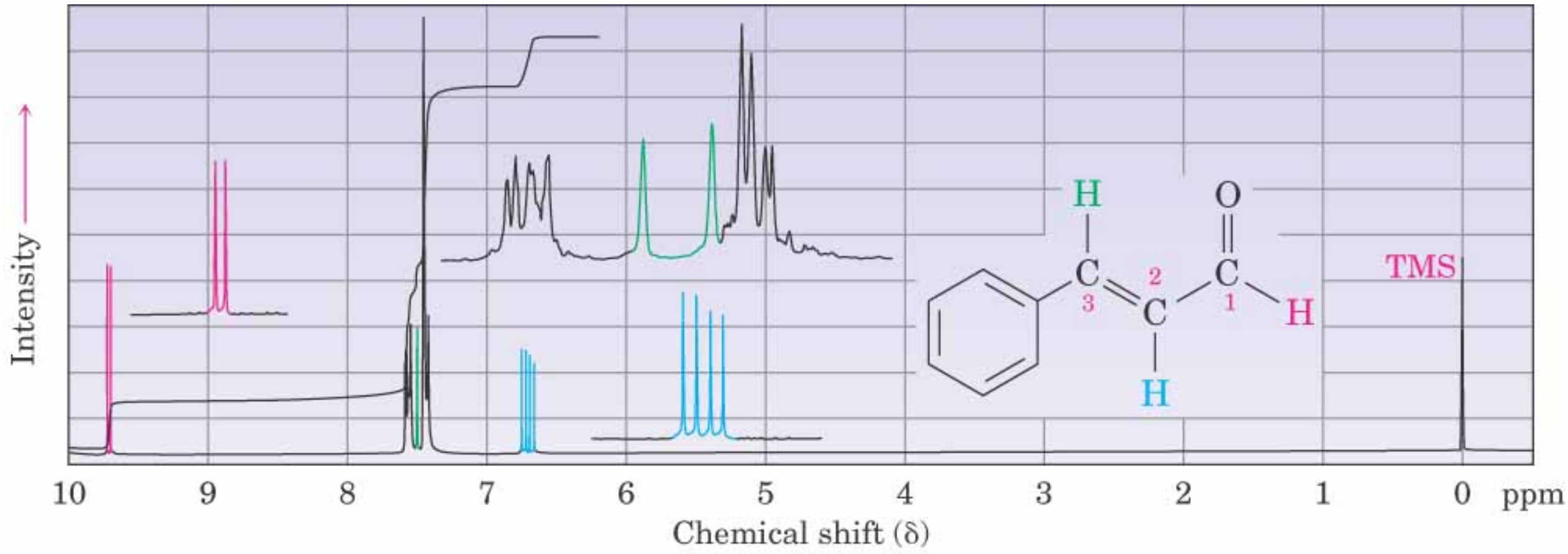




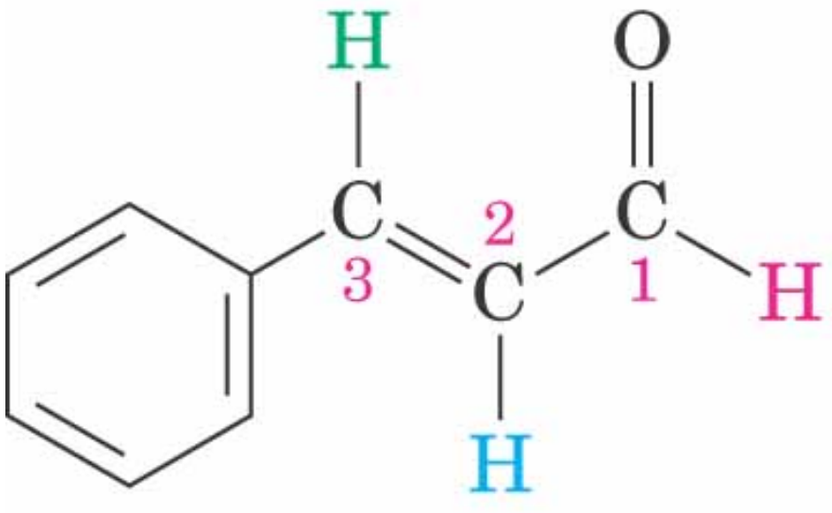


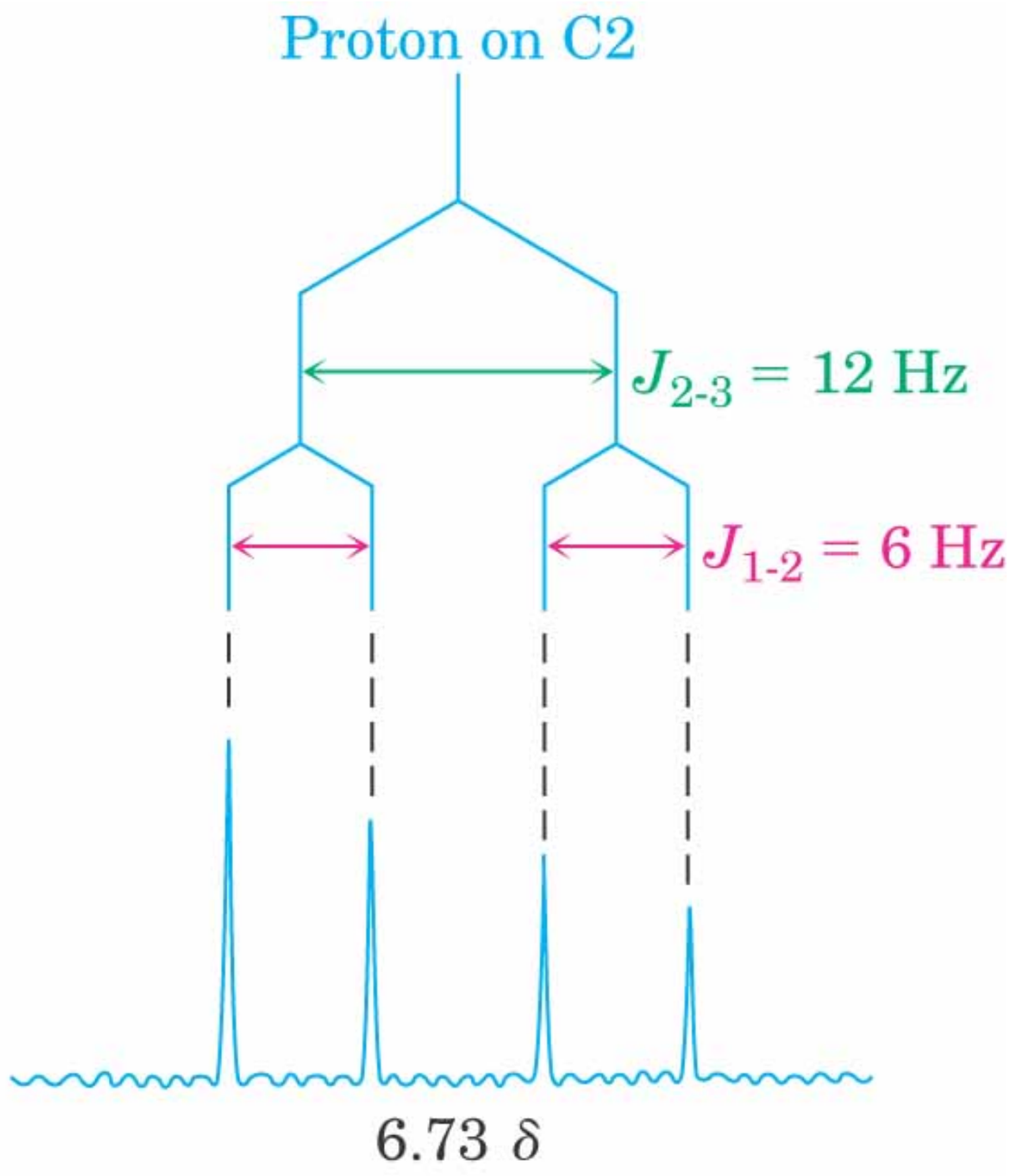
Cinnamaldehyde

- Multiple Coupling
- *J* H1-H2 = 6 Hz, H2-H3 = 12 Hz

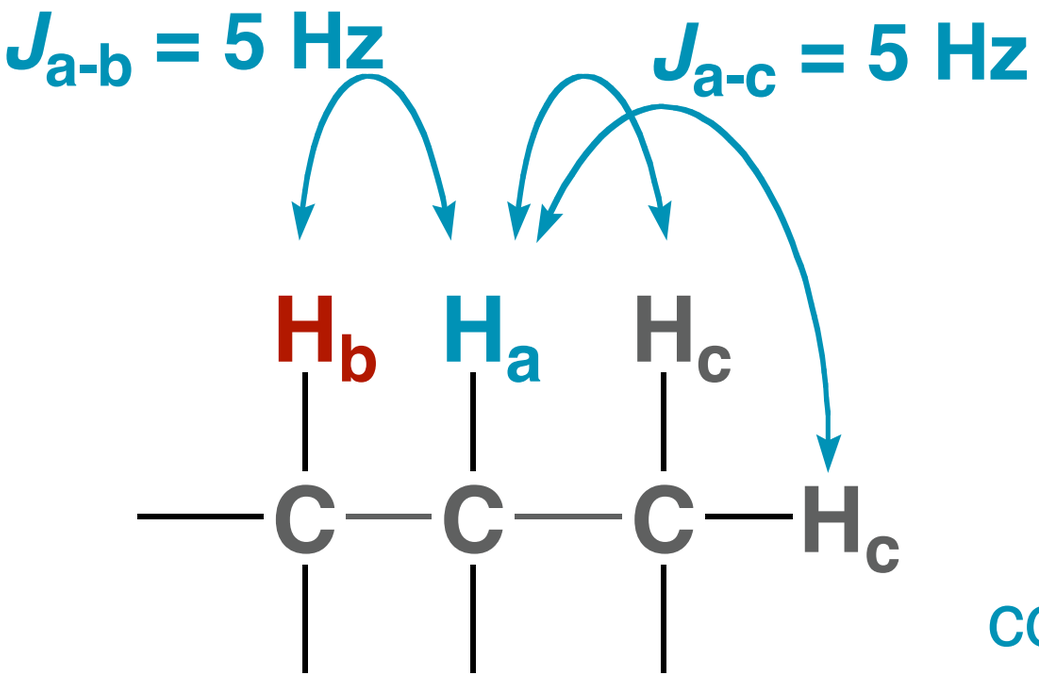


Cinnemaldehyde





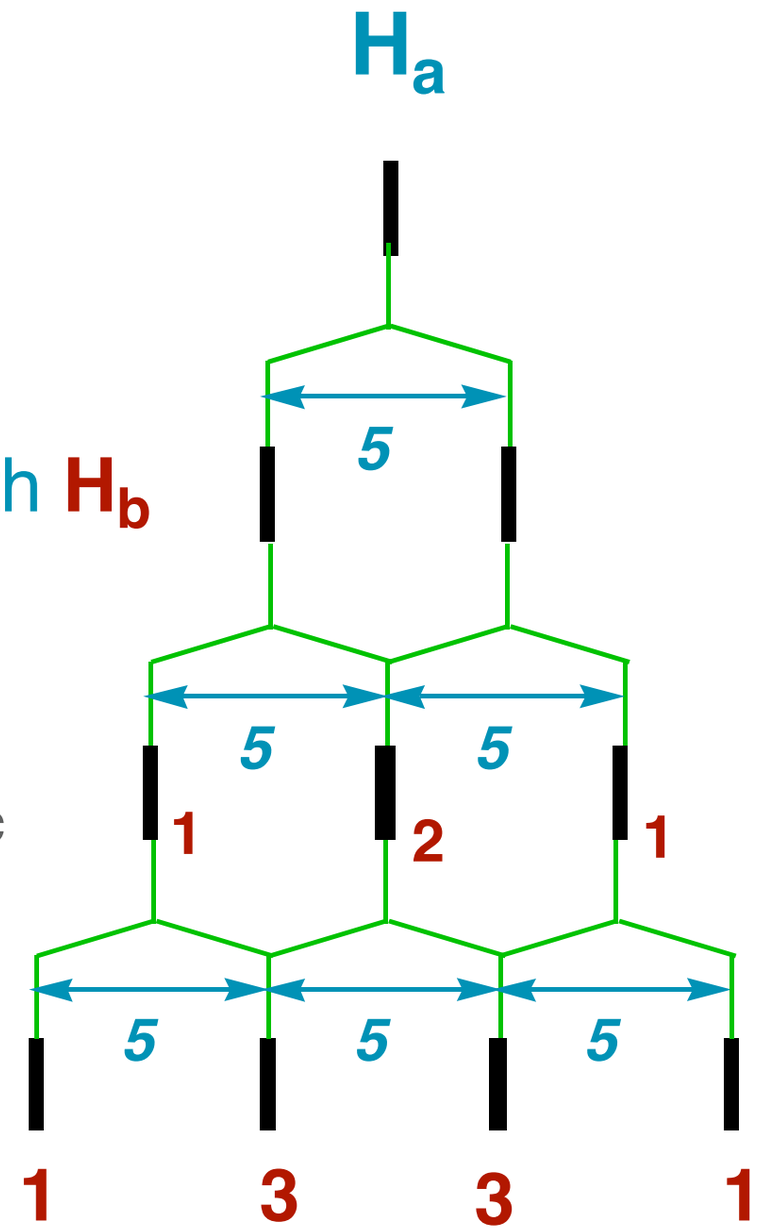
Multiple Coupling - Identical *J*



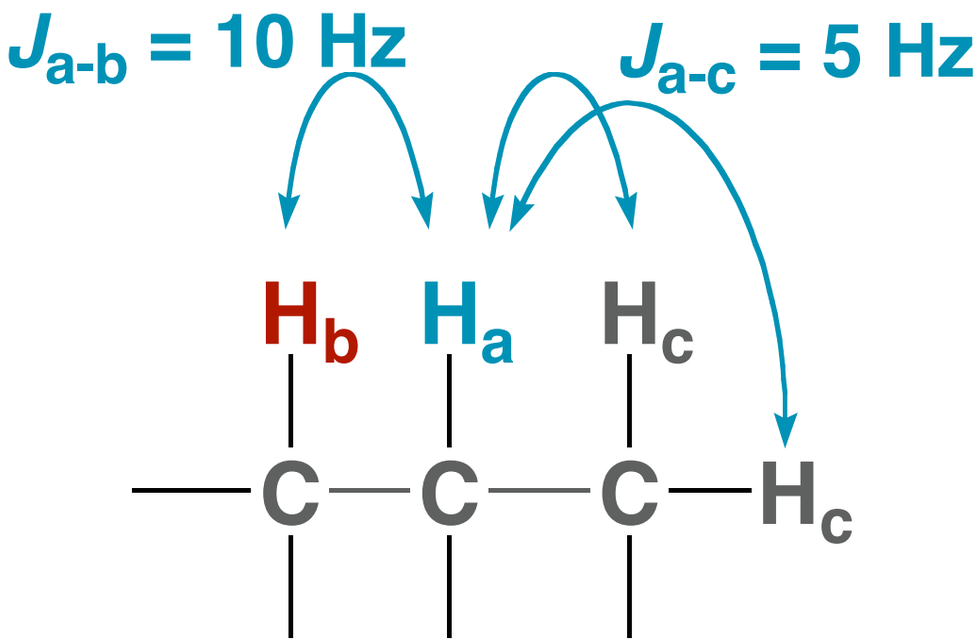
coupling with H_b

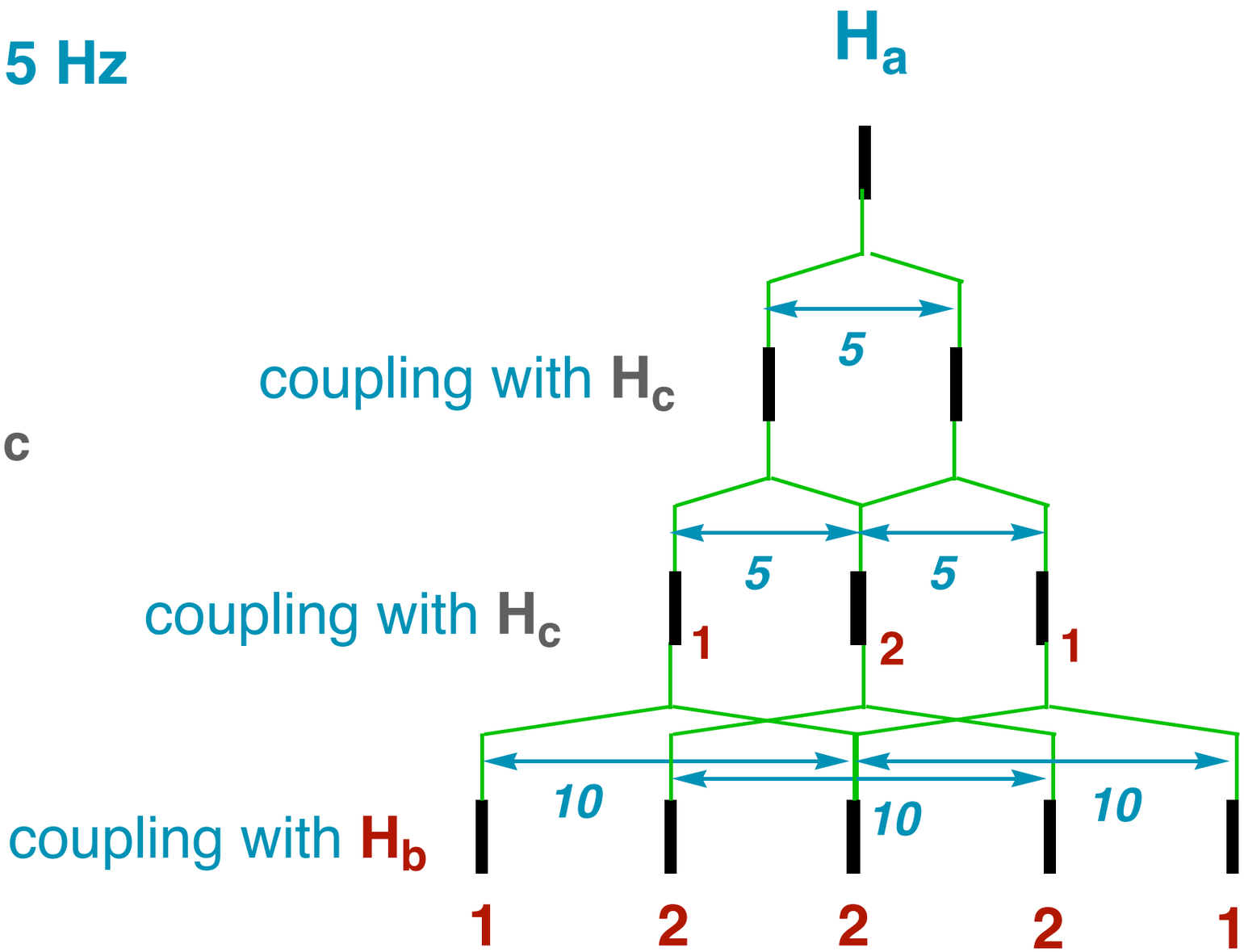
coupling with H_c

coupling with H_c

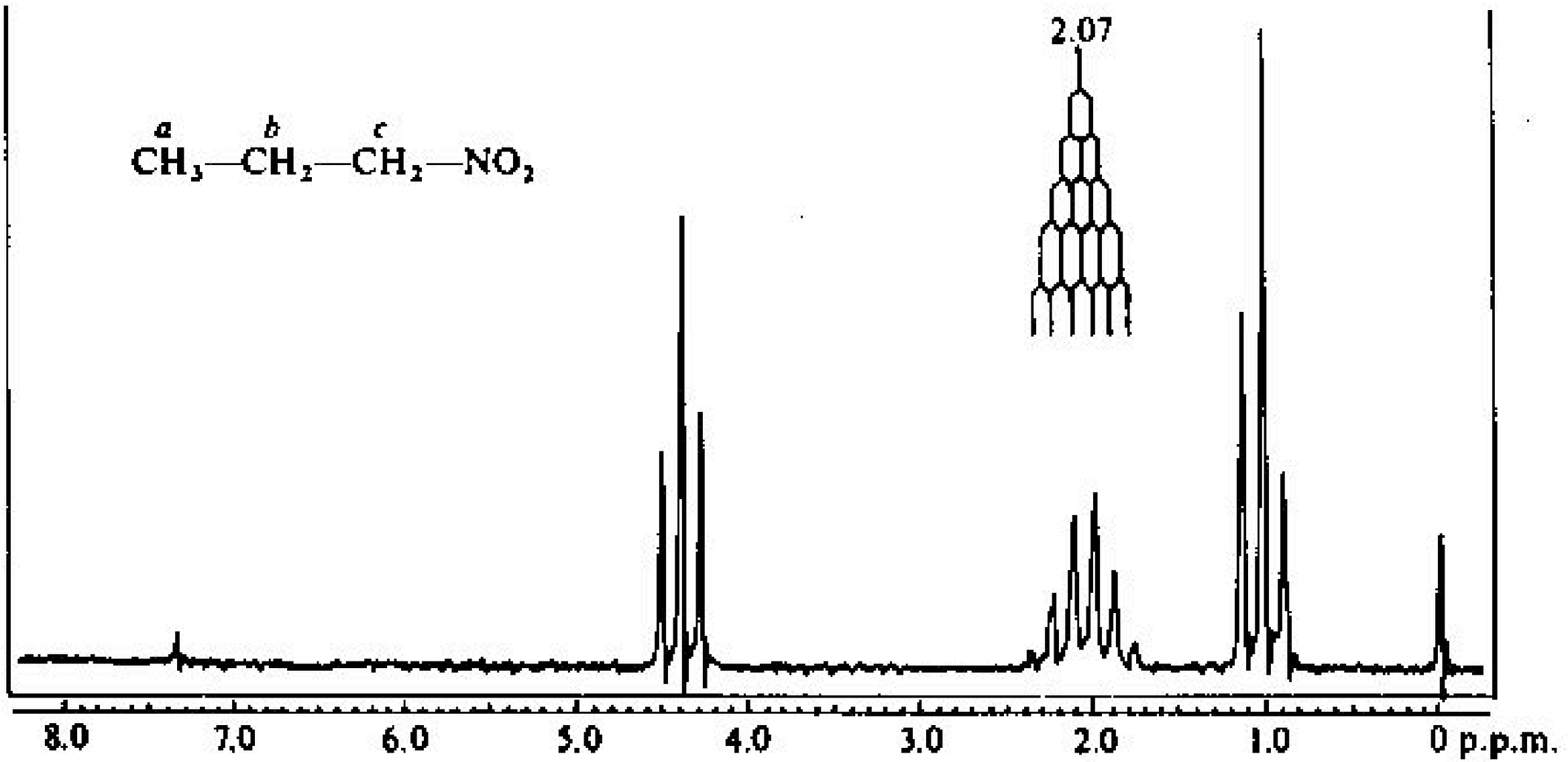


Multiple Coupling - Different *J*





Nitropropane



Strategies for Determining Unknows

- Given the Molecular Formula - calculate degrees of unsaturation.
- Identify functional groups
- Identify pieces of the structure
- Put the pieces together in a reasonable way
- Double check that your structure matches all the data given.

Degrees of Unsaturation

General Formula for Units of Unsaturation

$$UN = \frac{(2n+2) - \#H - \#X + \#N}{2}$$

2n+2 is the number of H's if completely saturated
#H is the actual number of H's in the molecule
#X is the actual number of halogens
#N is the actual numnber of nitrogens
divide by 2 because each unit of unsaturation removes 2 H's from the molecule

C_8H_8ClNO

$$UN = \frac{(16+2) - 8 - 1 + 1}{2} = \frac{10}{2} = 5$$