

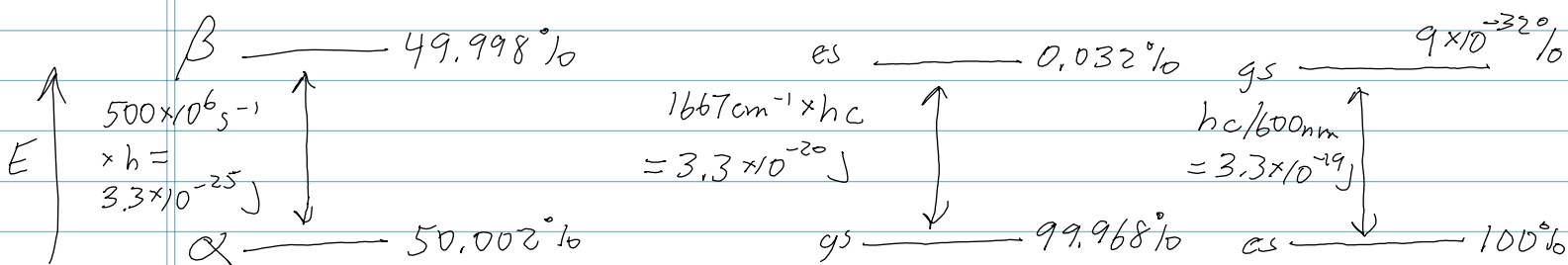
¹H NMR Splitting Patterns - 6 Things to Know

1) ~50% of all ¹H are in β state due to "thermal energy"

500 MHz NMR

cf) 1667 cm⁻¹ IR

600nm vis



Boltzmann: $\frac{P_{es}}{P_{gs}} = e^{-\Delta E/kT}$

$k = 1.38 \times 10^{-23} \text{ J/K}$

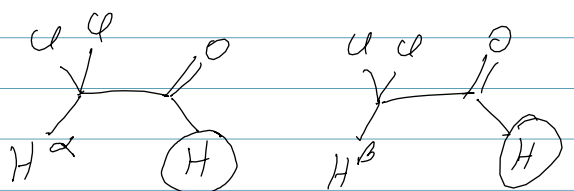
298 K

vibrational

electronic

2) Nearby ¹H (and other NMR nuclei) make their own fields (influence freq/field needed for resonance)

dichloroacetaldehyde



50.002%

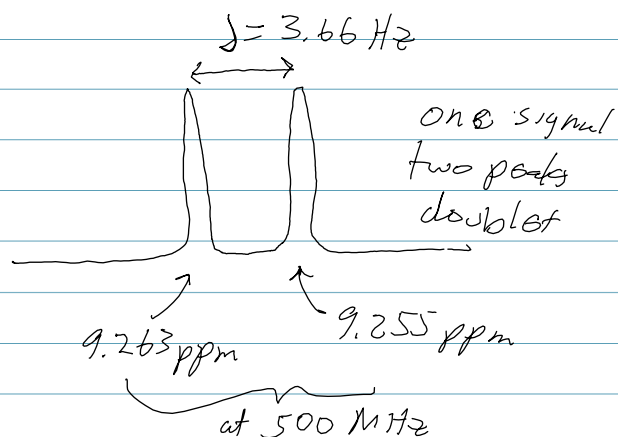
49.998%

downfield

upfield

(+ freq shift)

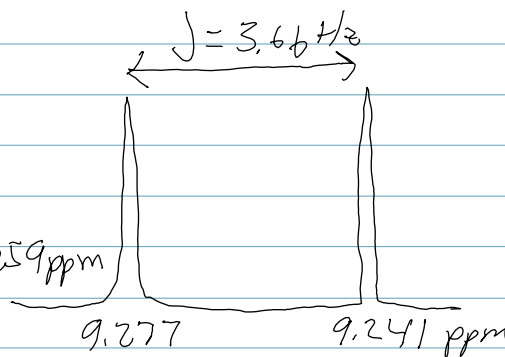
(- freq shift)



3) Splitting is in Hz not ppm

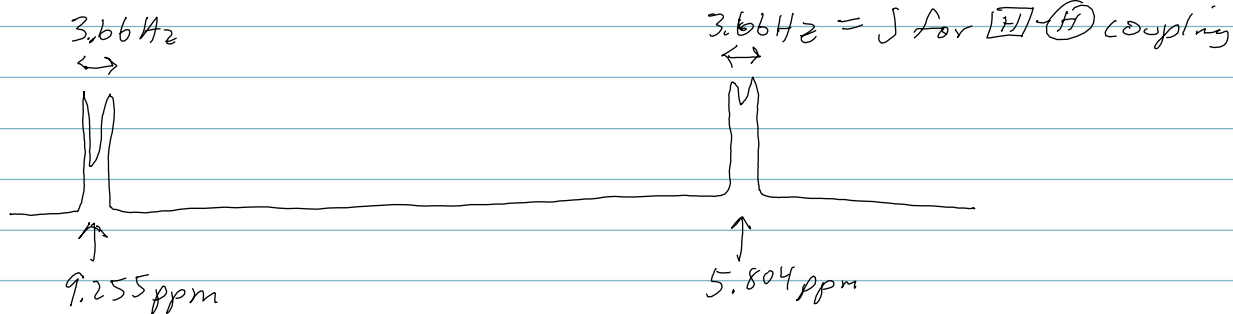
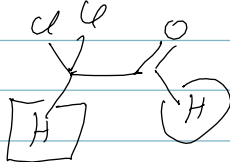
At 100 MHz

Report Avg δ of doublet peaks = 9.259 ppm



¹H NMR Splitting - 6 things to know (p2)

4) Splitting is the same both ways

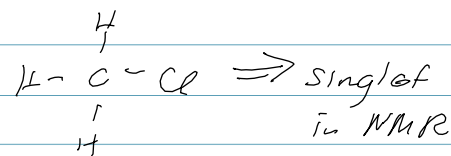


5) ¹H with same δ don't split each other.

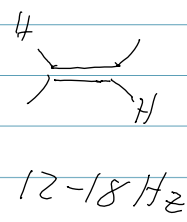
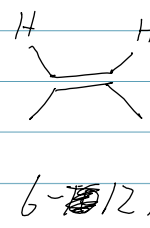
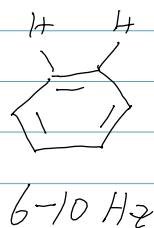
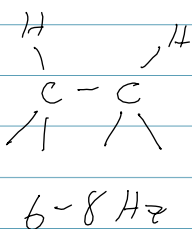
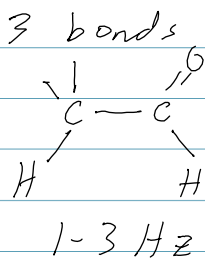
chemically equivalent

(or inequivalent

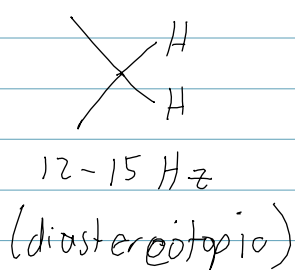
but accidentally have same δ)



6) Observable H-H splitting usually spans 2 or 3 bonds (sometimes 4)



2 bonds



4 bonds

