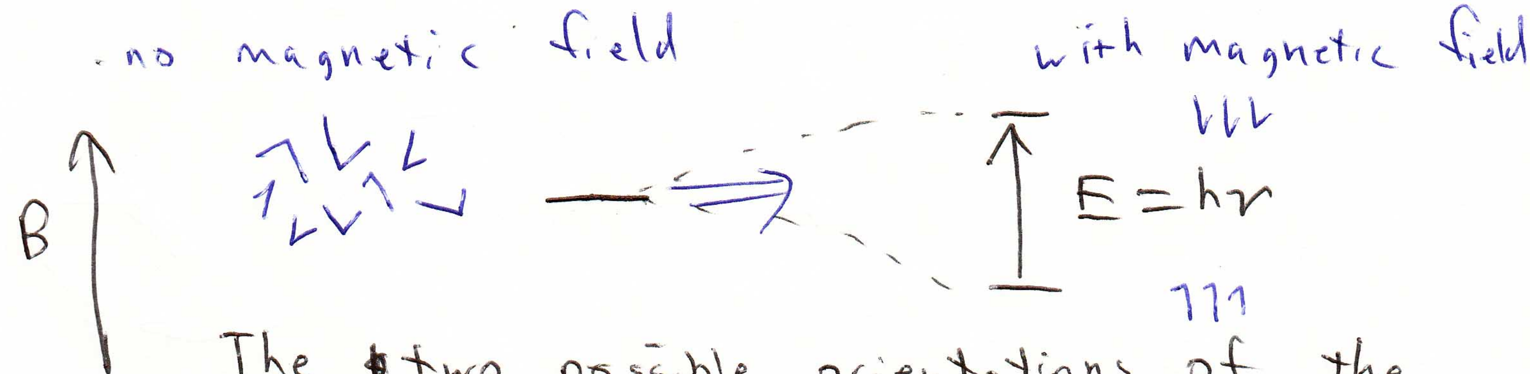
Nuclei have (usually) spin in much the same way that electrons have spin. For example, ^{1}H (protium) and ^{13}C have spin $\frac{1}{2}\hbar$. Nuclei with spin ½, when placed in a magnetic field, will align either parallel w/ the field or opposite the field.

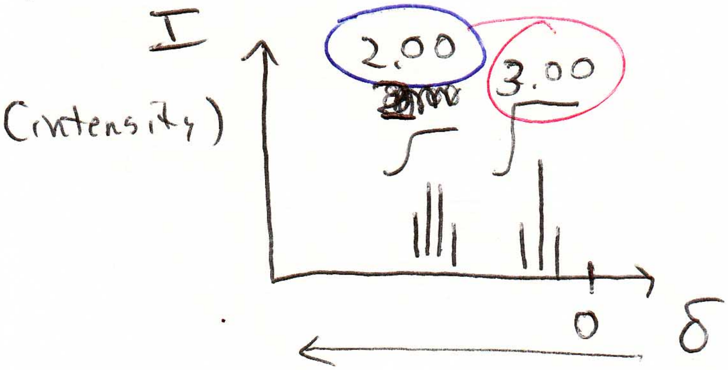


The two possible orientations of the nucleus create an energy gap, which can be crossed in a photon w/ the correct energy is absorbed. That photon corresponds to a specific frequency of light.

If a nucleus has an electron-withdrawing neighbor, that nucleus is more exposed to the magnetic field (deshielded), which causes a larger ΔE, which causes a high f of light to be absorbed.

$$\delta \equiv \frac{\text{observed frequency} - \text{machine } f}{\text{machine } f} \times 1{,}000{,}000$$

For ^{13}C + ^{1}H, TMS (tetramethylsilane) is used as the reference compound to determine the machine frequency.



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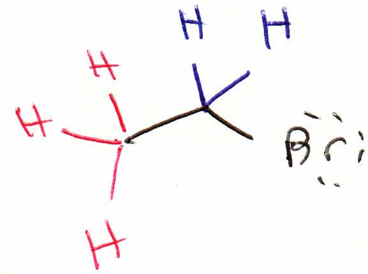
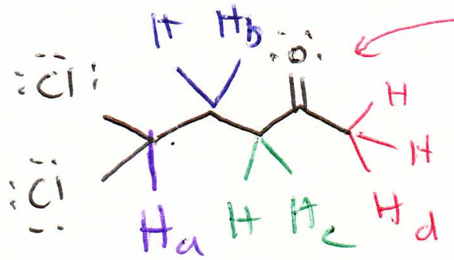


Valuable info:

1) Chemical shift – used to determine functional group
2) Integrals – Proportional to # of H
3) Splitting – Provides information about the # of neighbors.



C=O has no H on it, so it blocks splitting of the $-CH_3$.

δ 2.0, s, 3H

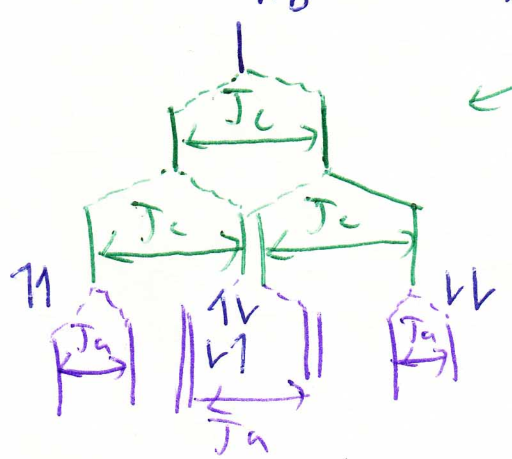
δ 5.3, t, 1H

δ 2.3, t, 2H

Splitting Tree

H_b δ 2.5, dt, 2H

splitting due to H_c



If $J_{bc} \gg J_{ab}$