

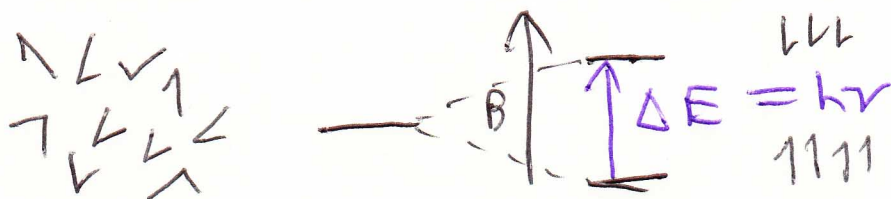
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Many nuclei have spin. For example,  $^1\text{H}$  (proton) and  $^{13}\text{C}$  have spin  $\frac{1}{2}$  [technically  $\frac{1}{2} \frac{h}{2\pi} = \frac{1}{2} \hbar$ ]. Nuclei with spin are randomly arranged in the absence of a magnetic field; in the presence of a magnetic field, nuclei with spin  $\frac{1}{2}$  can align either with the magnetic field or against it. This causes an energy gap to form.

no magnetic field

w/ mag. field

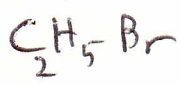


If a photon with the correct energy (which corresponds to light of a particular frequency) is absorbed by the nucleus, the nucleus can flip from the low- to high-energy spin state. The energy released when the nucleus returns to the lower state is measured by an NMR spectrometer.

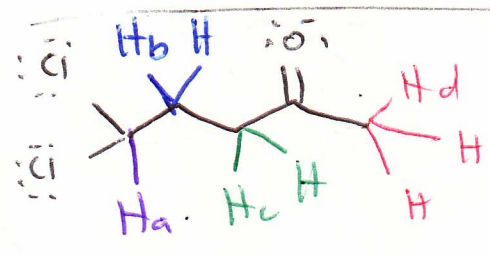
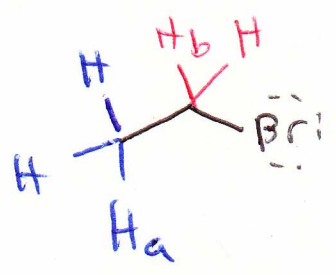
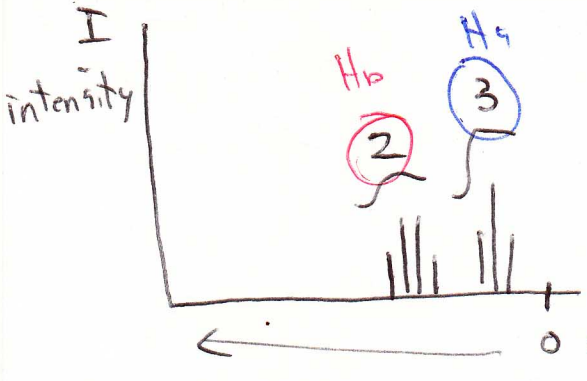
If a nucleus has an electronegative neighbor, that neighbor will pull electron density away from the nucleus (deshield), exposing the nucleus more greatly to the magnetic field. This causes a larger energy gap, which means a higher frequency of light would be needed.

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

For  $^1\text{H}$  and  $^{13}\text{C}$ , the machine frequency is determined by using the reference standard TMS (tetramethylsilane).



- chemical shift  $\rightarrow$  functional group
- integration  $\rightarrow$  proportion to the # of H's.
- splitting  $\rightarrow$  gives information about neighbors



- $\delta$  2.0, s, 3H
  - $\delta$  2.3, t, 2H
  - $\delta$  2.5, dt, 2H
  - $\delta$  5.3, t, 1H
- If  $J_{ab} \ll J_{bc}$

