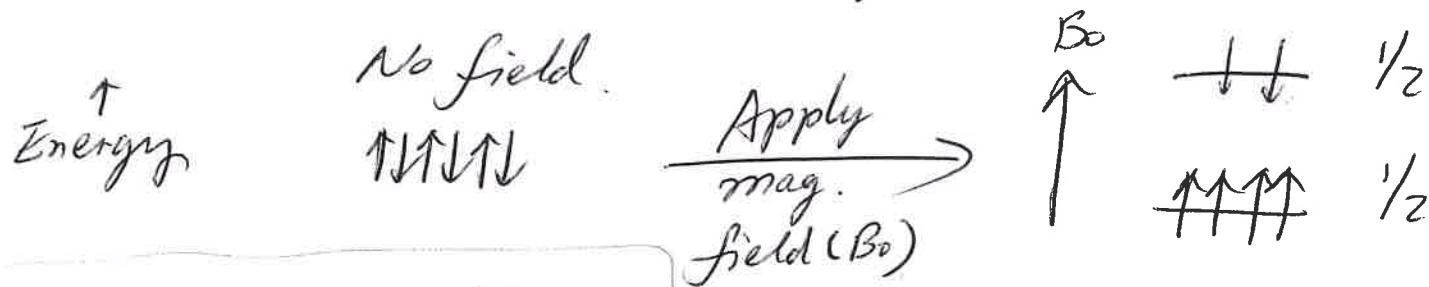


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Recall: NMR - measurement based on nuclear spin
 ^1H nuclei have 2 spin states, $+\frac{1}{2}$ (\uparrow) & $-\frac{1}{2}$ (\downarrow). In a magnetic field, these states have different energies
 \rightarrow basis of NMR spectroscopy.



Infrared (radio freq) $h\nu$ \Rightarrow characteristic frequency for "spin flip"
 The diagram shows two energy levels with arrows indicating a transition between them, corresponding to the energy $h\nu$ and the characteristic frequency for a spin flip.

Energy required for H spin flip depends on "local environment" w/in a molecule.

Non-equivalent H's are in different local environments.

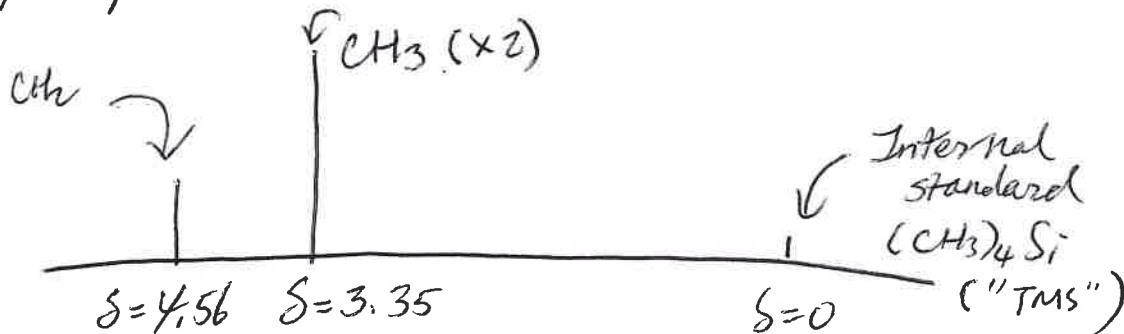
Example:



2 kinds of H: CH_3 kind (6) . CH_2 kind (2)

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^1H spectrum:



Horizontal scale:

Relative measurement (not affected by mag. field differences); referenced to the internal standard (TMS).

Note: δ vs. ppm (parts per million).

Thus, $\delta = 4.56 \equiv 4.56 \text{ ppm}$.

There is no vertical scale.

However, for ^1H NMR, the integration of area under signal is proportional to ratio of H's that contribute to the signals.

Thus, for $\text{CH}_3\text{-O-CH}_2\text{-O-CH}_3$,

$$\delta = 4.56$$

$$\delta = 3.35$$

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δ	Rel integration	
$\delta = 4.56$	1	} Consistent w/ 6:2 for $\text{CH}_3:\text{CH}_2$
$\delta = 3.35$	3	

Position of an NMR resonance is as the "chemical shift" for that resonance \rightarrow How interpret chemical shift?

One major factor that influences ^1H chemical shifts: electronegativity of nearby atoms. Increasing nearby electronegativity negative atoms \Leftrightarrow large δ .

From Table 13.1

	δ
$\text{H}_3\text{C}-\text{F}$	4.26
$\text{H}_3\text{C}-\text{Cl}$	3.05
$\text{H}_3\text{C}-\text{C}(\text{CH}_3)_3$	0.86
$\text{H}_3\text{C}-\text{Si}(\text{CH}_3)_3$	0 [TMS, by definition]

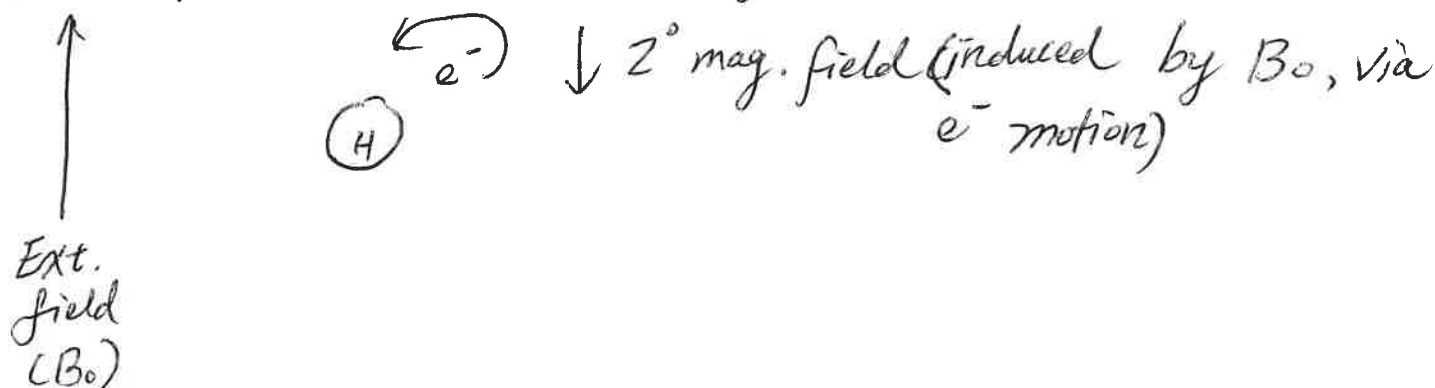
physical origin of this δ trend?

External mag. field. Causes motion of e^- 's w/in the molecule, thereby creating a secondary mag. field

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that opposes the external field.

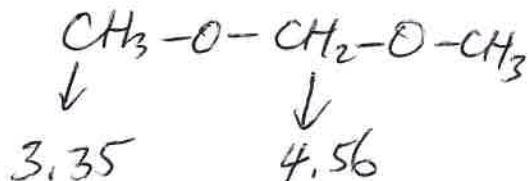


more e^- density around a given H nucleus \Rightarrow large 2° mag. field. \Rightarrow "more shielding" (i.e. smaller net mag. field "felt" by that H nucleus \rightarrow smaller δ (closer to TMS)).

Electronegative atom nearby \Rightarrow less e^- density around H \Rightarrow larger δ .

$\text{CH}_3\text{-F}$ $\text{CH}_3\text{-Cl}$
 $\delta = 4.26$ vs. ~~$\delta = 3.05$~~

Recall: [see Appendix 3.]



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Multiplicity of NMR signals.

Consider $\text{CH}_3\text{CH}_2-\text{O}-\text{CH}_2\text{CH}_3$

6 CH_3 H's

4 CH_2 H's

