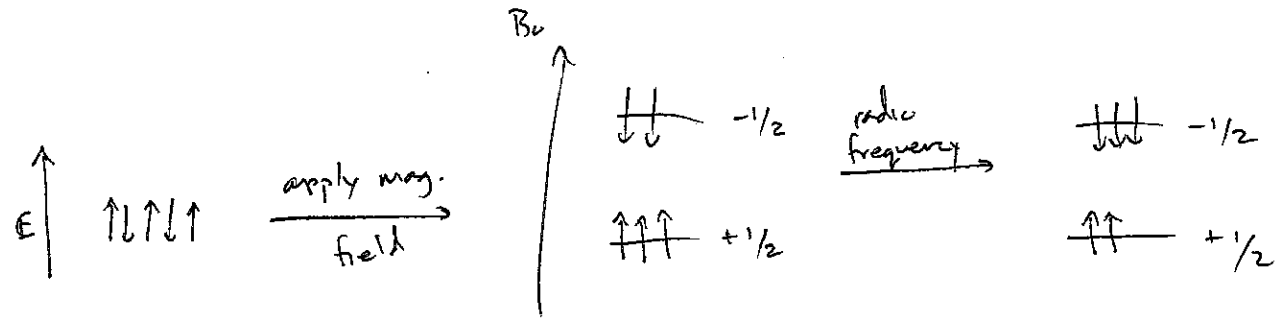


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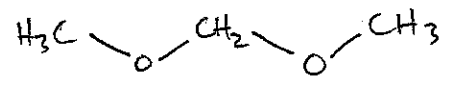
Recall: NMR measurement detects difference between two spin states  
 - this energy is distinct for each type of H



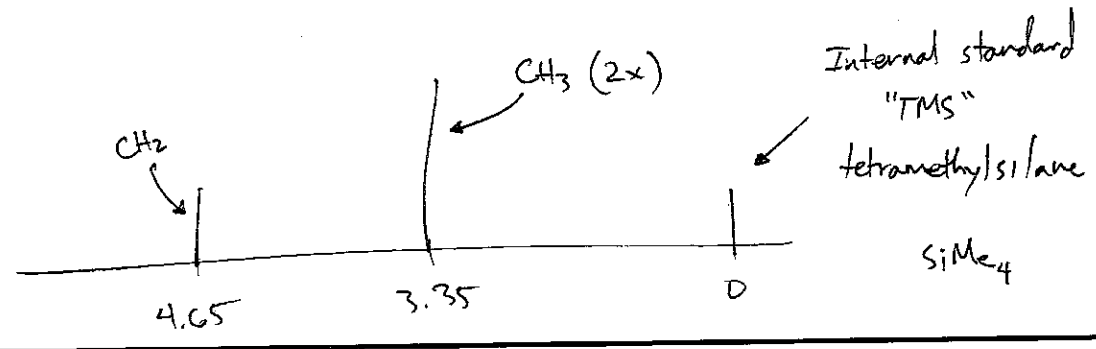
• NMR experiment:

- place sample in strong magnetic field
- hit sample with sweep of radio frequencies
- record frequencies the sample absorbs at.

• Ex: (Fig B.3)



- 2 types of H's



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NMR is plotted:

1) Horizontal scale

- expect frequency

- frequency for NMR depends on strength of  $B_0$ .

• Two methods to get around this:

• 1) measure difference relative to TMS (at 0 ppm)

2) divide difference by "operating frequency"

↓ result

horizontal scale has no physical units

small → "parts per million" or "ppm"

• Horizontal scale: position in NMR spectrum depends on local environment of each nucleus

→ "chemical shift" ( $\delta$ )  $\delta = 4.56$  or  $4.56$  ppm

2) Vertical scale

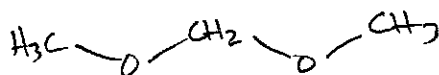
- no specified unit

- relative intensities of peaks are proportional to # of H's giving signal

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ratio of integrations  $\approx$  ratio of H's

back to example:



	<u>rel. integration</u>	
$\delta$ 4.56 ( $\text{CH}_2$ )	1	i.e.: 2 vs 6
$\delta$ 3.35 ( $2 \times \text{CH}_3$ )	3	

### Chemical shift ( $\delta$ )

- $\delta$  for a given H is a characteristic of local environment
- many factors that influence chemical shift

\* DO PRACTICE PROBLEMS TO UNDERSTAND THIS \*  
 (Tables in Appendix 3)

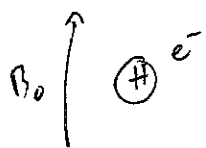
One major factor that influences  $\delta$  is electronegativity of nearby atoms

Ex:		<u><math>\delta</math></u>
	$\text{H}_3\text{C}-\text{F}$	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

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• Origin of electronegativity's effect on  $\delta$ :

- nearby  $e^-$ 's influence the overall magnetic field  
"felt" by H



the magnetic field induced by  $e^-$  motion  
reduces the strength of the field that  
the H feels

"shielding"

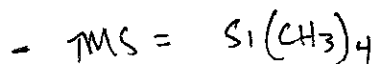
• More  $e^-$  density at H: more shielding

→ resonances are more to the right (smaller  $\delta$ )

• Less  $e^-$  density (i.e.  $\nearrow$  near an electronegative element)

→ resonances are more to the left (larger  $\delta$ )

• TMS as standard:

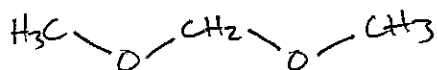


Si has low electronegativity  $\Rightarrow$  low  $\delta$

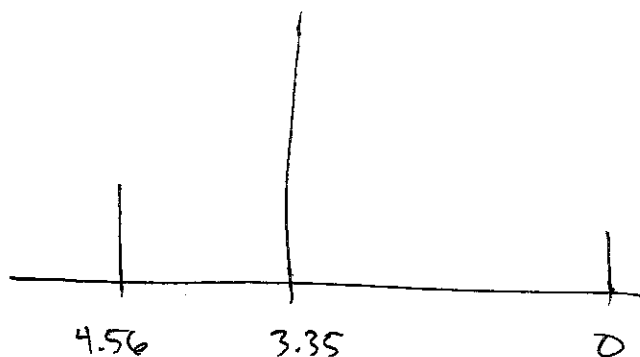
• most organic molecules (their H's) occur to the left of TMS

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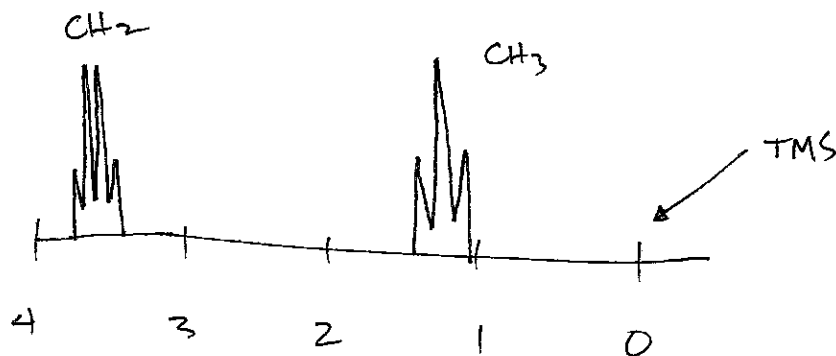
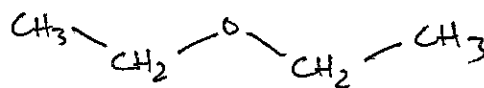
back to this guy....



"downfield"  
(left)

"upfield"  
(right)

• Contrast to diethyl ether:



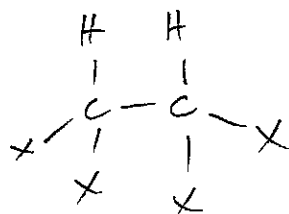
• new phenomenon: the signals in this molecule are being split into multiple peaks

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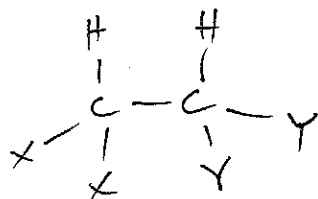
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- "splitting" of H resonance arises when nearby, non-equivalent H's influence the local magnetic field

Examples:



the two H's are equivalent  $\Rightarrow$  1 peak



$\Rightarrow$

- the two H's are non-equivalent
- 2 ~~≠~~ signals in  $^1\text{H}$ NMR
- each signal will be split into two peaks (due to presence of nearby H)