

(14) **Today**

Chap 13: Nuclear Magnetic Resonance Spectroscopy

**Next Class** (15)

Chap 13: Nuclear Magnetic Resonance Spectroscopy

(16) **Second Class from Today**

Chap 13: Nuclear Magnetic Resonance Spectroscopy

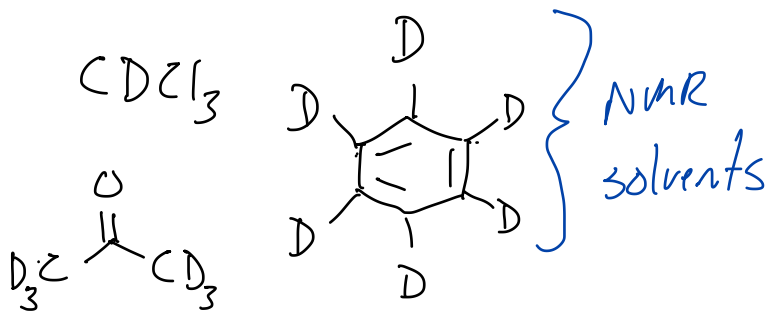
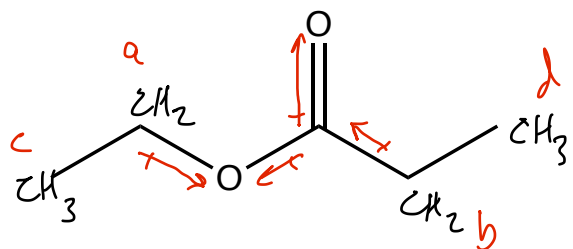
**Third Class from Today** (17)

Chap 12: Infrared Spectroscopy

Spring Break Begins at 4:30

Test is not graded yet :-(

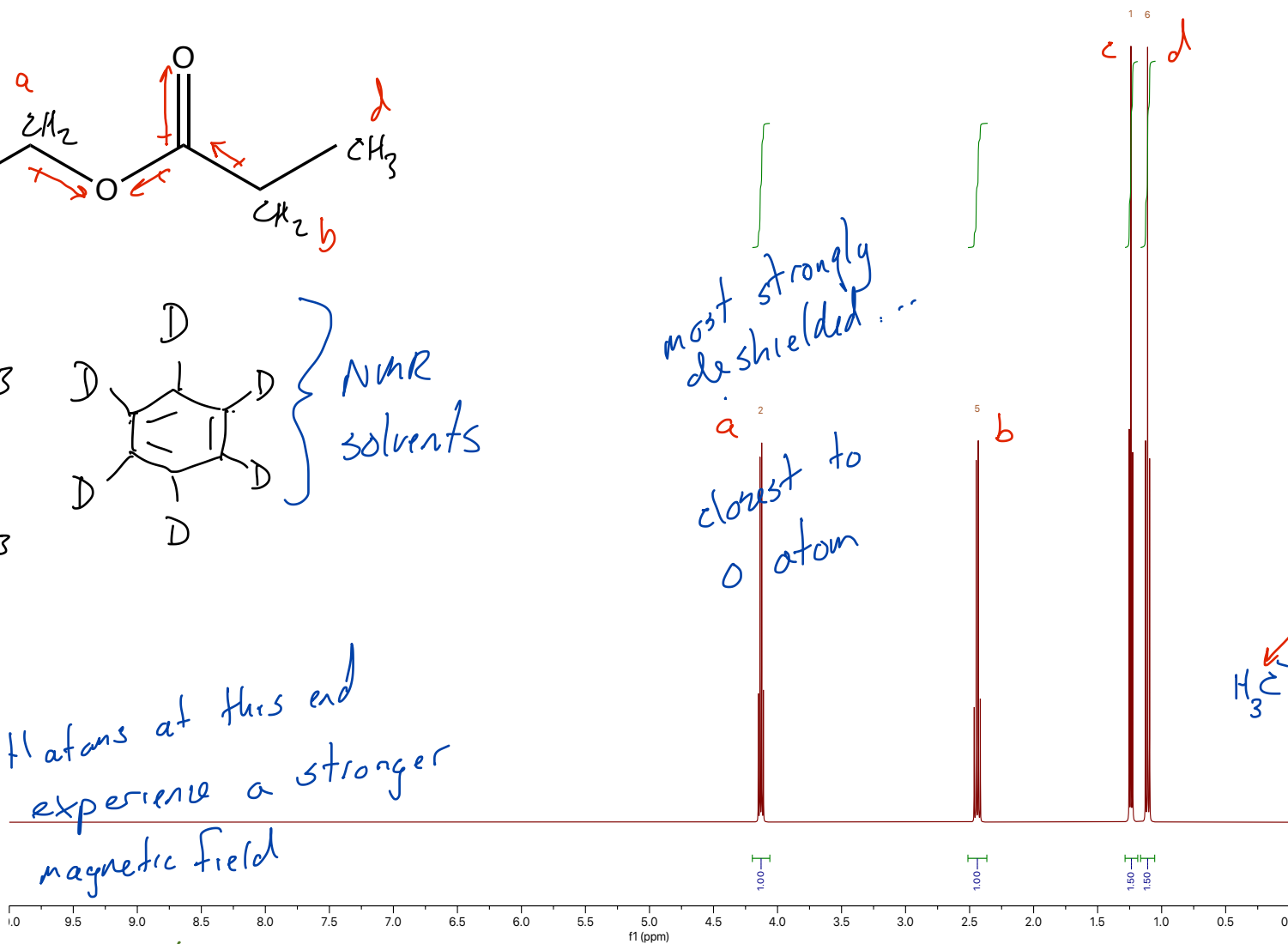
# Why Are Some Further to the Left or Right?



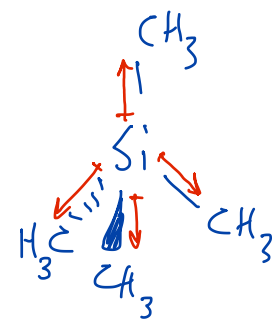
Protons at this end experience a stronger magnetic field

"H's out here experience a stronger field because they are "deshielded"

most strongly deshielded...  
closest to O atom



The <sup>1</sup>H atoms in TMS are in a e<sup>-</sup> rich environment  
e<sup>-</sup>'s interfere with the magnetic field

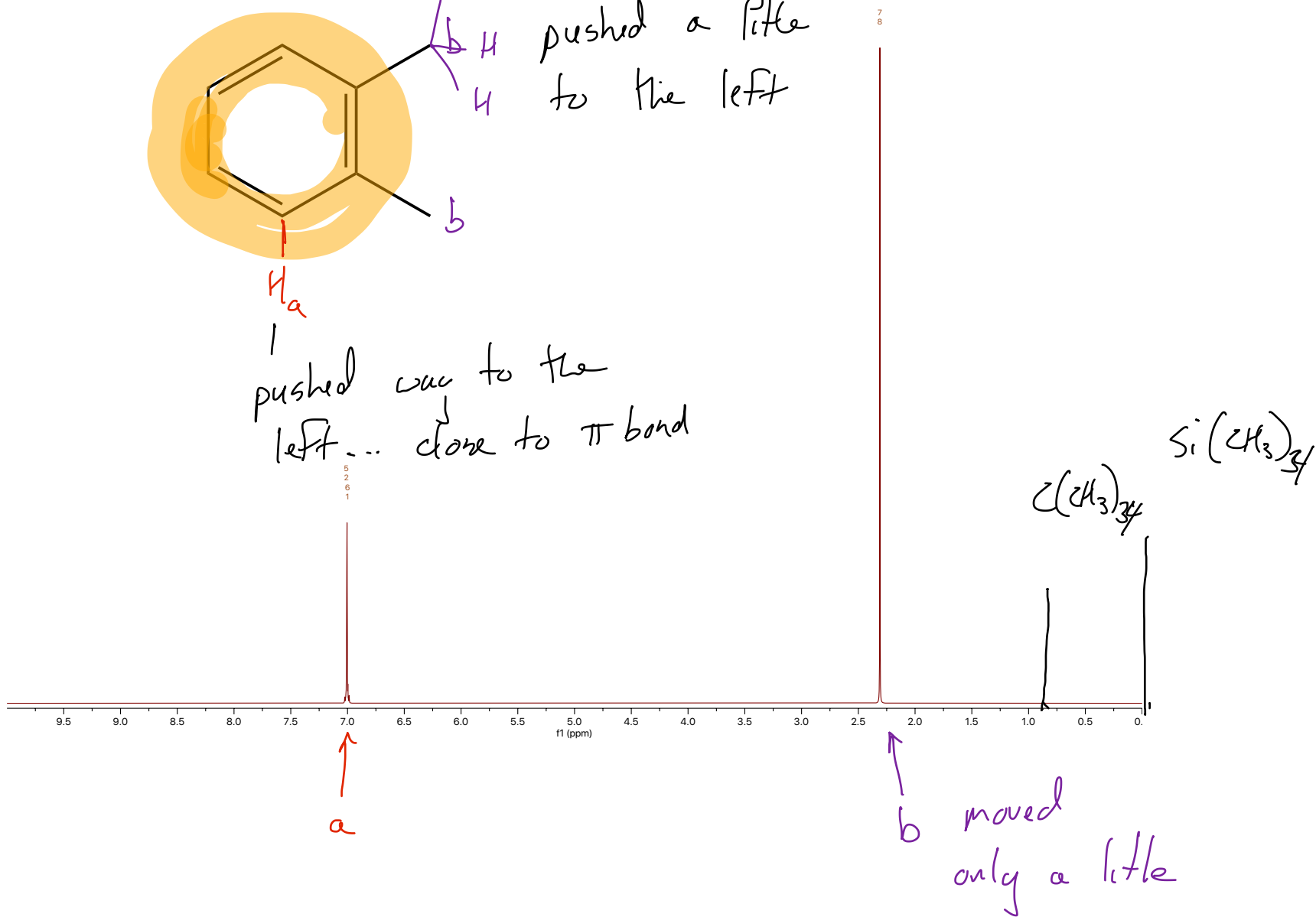
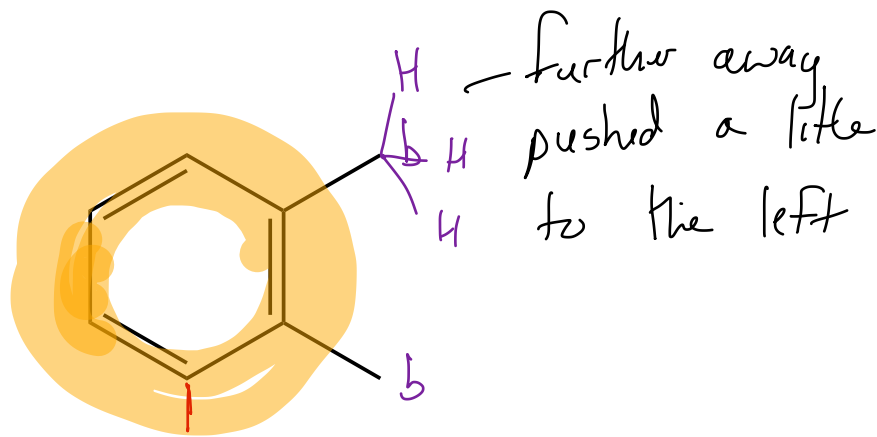


these H's

experience a weak field because they are shielded by the e<sup>-</sup>

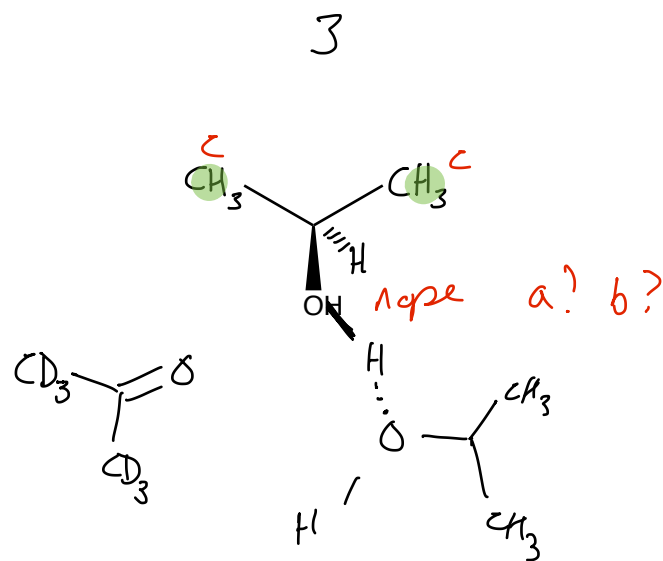
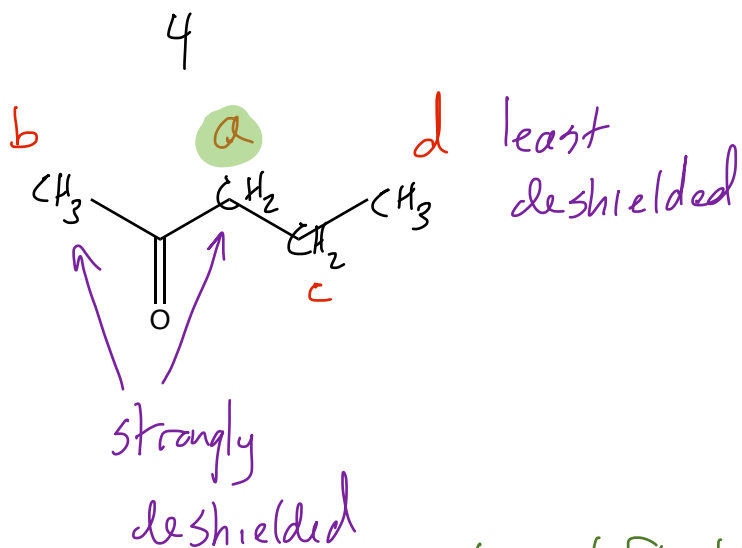
# Why Are Some Further to the Left or Right?

Predicted <sup>1</sup>H NMR Spectrum

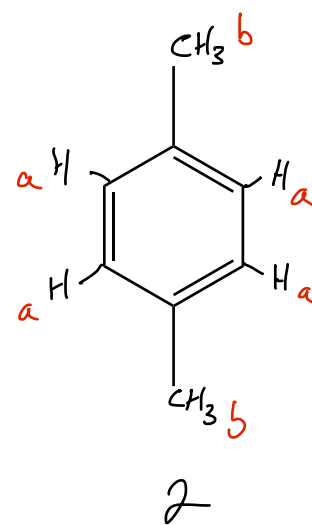
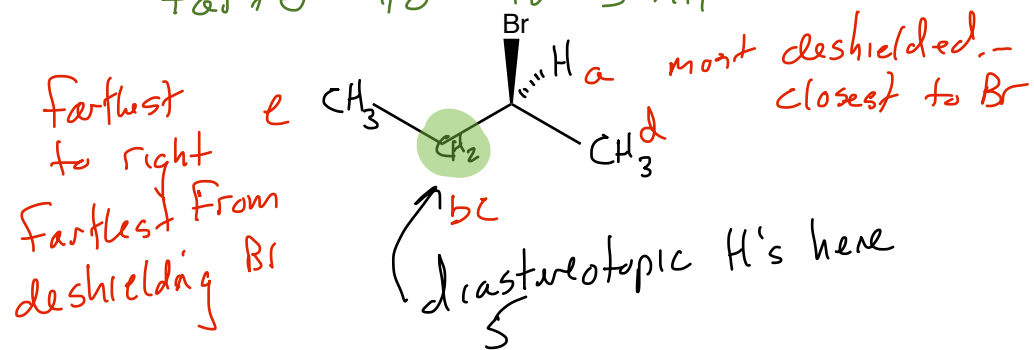


## Why Some Further to the Left or Right?

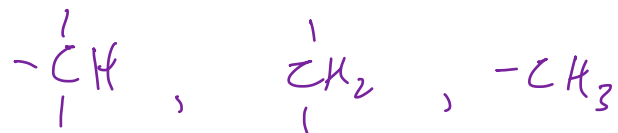
Practice: How many peaks? Assign letters alphabetically based on expected position in the NMR spectrum: **A** farthest to the left, **B** first peak to the right of A, etc.



CH<sub>2</sub>'s start further to the left than CH<sub>3</sub>'s, so if the C=O pushes them to the left, the CH<sub>2</sub> will wind up further to the right

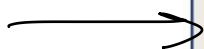


# Characteristic Chemical Shifts



1.4                  1.2-3                  0.9

not exact values  
use as a guide



**Table 14.1 Approximate Values of Chemical Shifts for <sup>1</sup>H NMR<sup>a</sup>**

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
(CH <sub>3</sub> ) <sub>4</sub> Si	0		6.5-8
-CH <sub>3</sub>	0.9		9.0-10
-CH <sub>2</sub> -	1.3	I-	2.5-4 <i>1.6</i>
	1.4	Br-	2.5-4
-C=C-CH <sub>3</sub>	1.7	Cl-	3-4
	2.1	F-	4-4.5
	2.3	RNH <sub>2</sub>	Variable, 1.5-4
-C≡C-H	2.4	<b>ROH</b>	<b>Variable, 2-5</b>
R-O-CH <sub>3</sub>	3.3	ArOH	Variable, 4-7
R-C=CH <sub>2</sub>	4.7		Variable, 10-12
R-C=C-H	5.3		Variable, 5-8

*CH ~ 3.8 ppm*

<sup>a</sup>The values are approximate because they are affected by neighboring substituents.