Today

Section 14.1 - 14.9
Introduction to Nuclear Magnetic Resonance, Shielding, Chemical Shift, and Integration

Next Class

Section 14.1 - 14.9
Introduction to Nuclear Magnetic Resonance, Shielding, Chemical Shift, and Integration

Section 14.10 - 17
Splitting and Multiplicity

Second Class from Today

Section 14.20
13C {1H} NMR

Practice Determining Structure Based on Spectroscopic Data

Third Class from Today

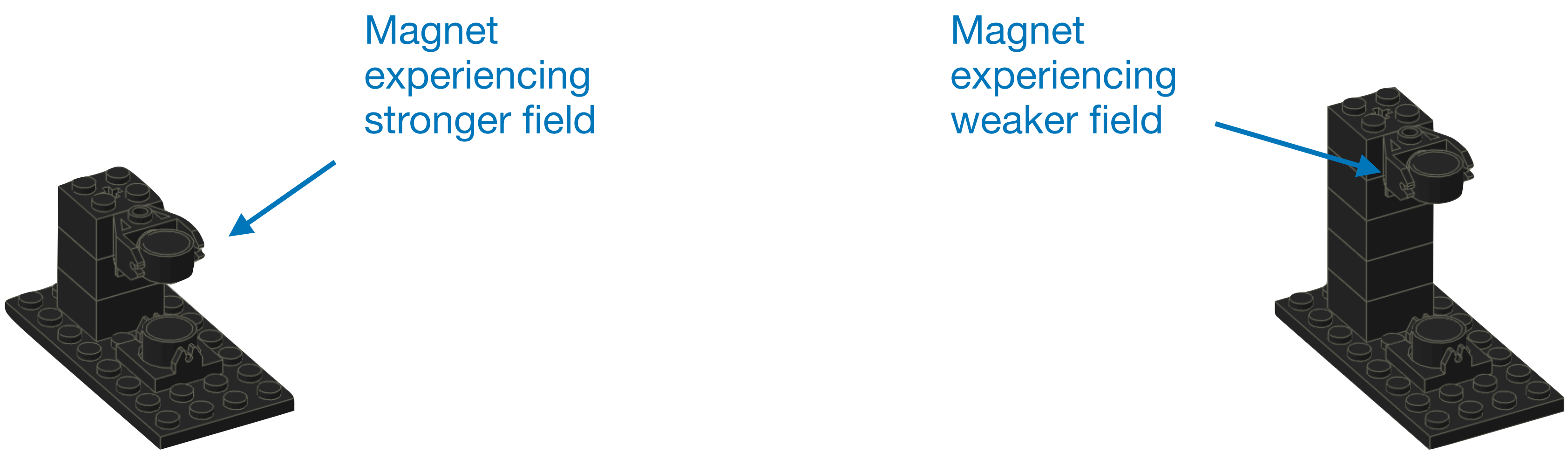
Chapter 15
Carbonyl Chemistry

NMR Introduction

When a magnet is placed in a magnetic field the magnet will align with the field.

When perturbed the magnet will resonate until it returns to its equilibrium position.

The frequency of the resonance depends on the strength of the magnetic field: a strong magnetic field will cause a high frequency resonance.



When a magnet is placed in a magnetic field the magnet will align with the field.

When perturbed the magnet will resonate until it returns to its equilibrium position.

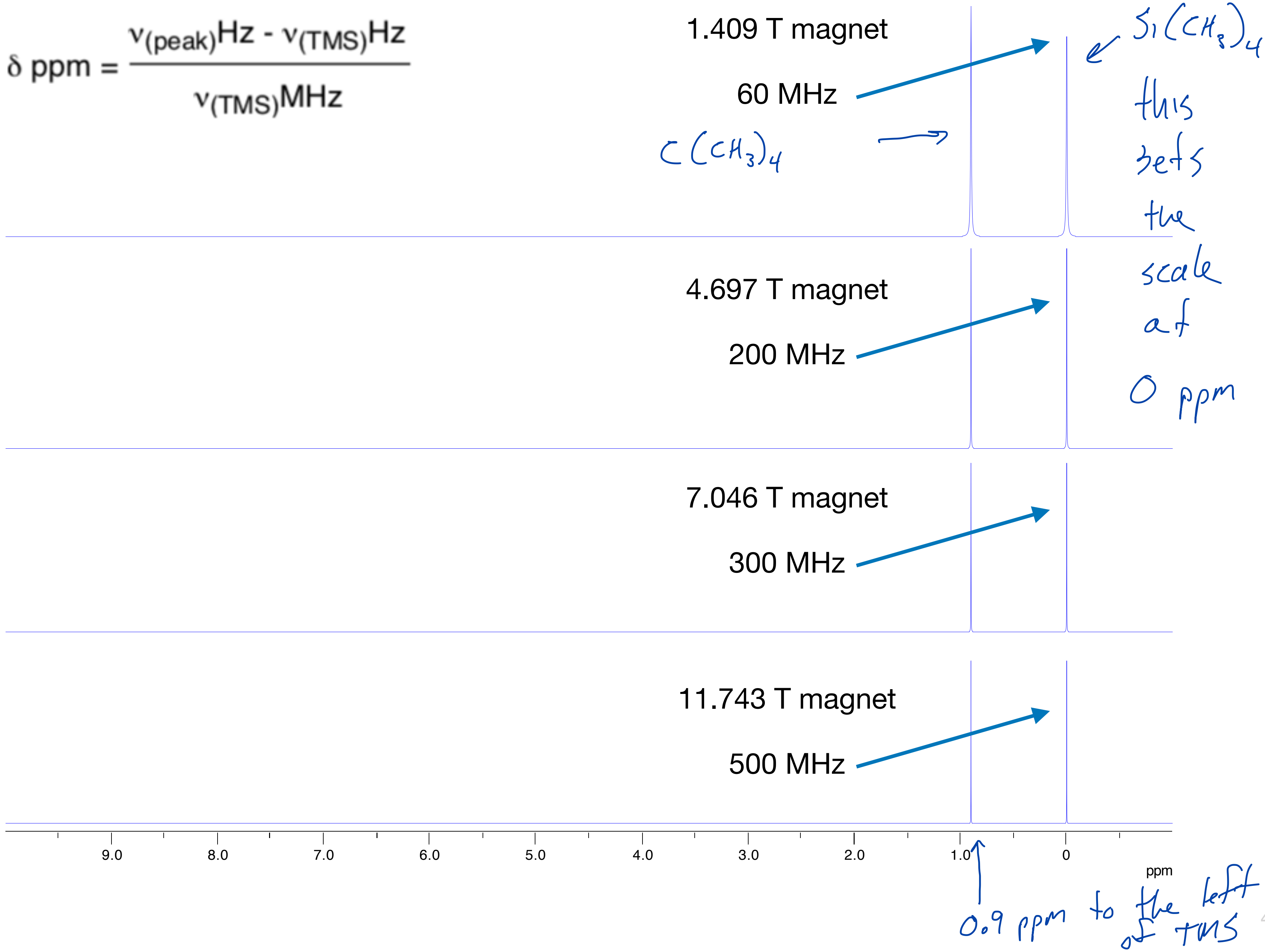
The frequency of the resonance depends on the strength of the magnetic field: a strong magnetic field will cause a high frequency resonance.

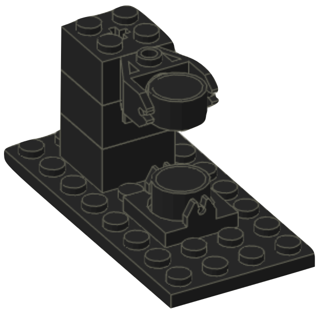
^{1}H are very weak magnets. When placed in a strong magnetic field, some of them align with the field.

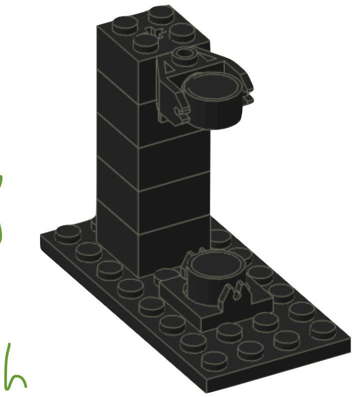
The alignment can be perturbed using radio waves.

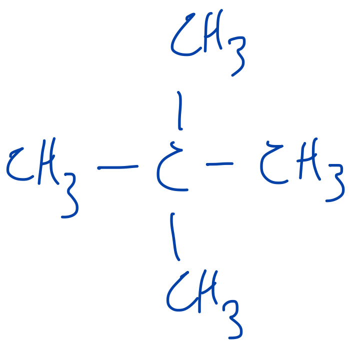
The perturbed (excited) ^{1}H atoms can be observed using radio waves as they resonate while returning to their equilibrium positions (relaxing back to their ground state).

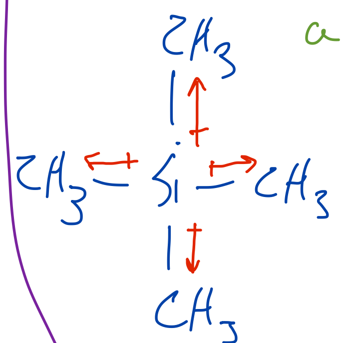
$$\delta \text{ ppm} = \frac{\nu_{(peak)}\text{Hz} - \nu_{(TMS)}\text{Hz}}{\nu_{(TMS)}\text{MHz}}$$





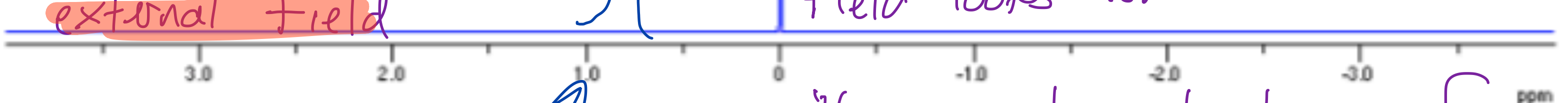






these H's must be experiencing a lower strength magnetic field because they are resonating at a lower frequency

CH_3's + ∴ the ¹H on $Si(CH_3)_4$ are in a more e⁻ rich environment.... and the e⁻'s create magnetic fields that shield the ¹H's from the external field



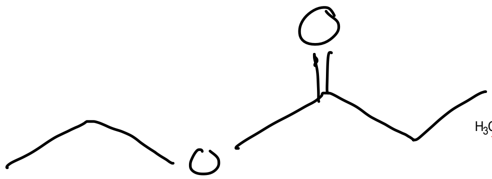
Field looks lower...

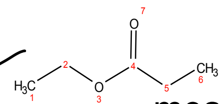
¹H resonate at lower freq

high freq

The NMR Spectrum

Predicted 1H NMR Spectrum



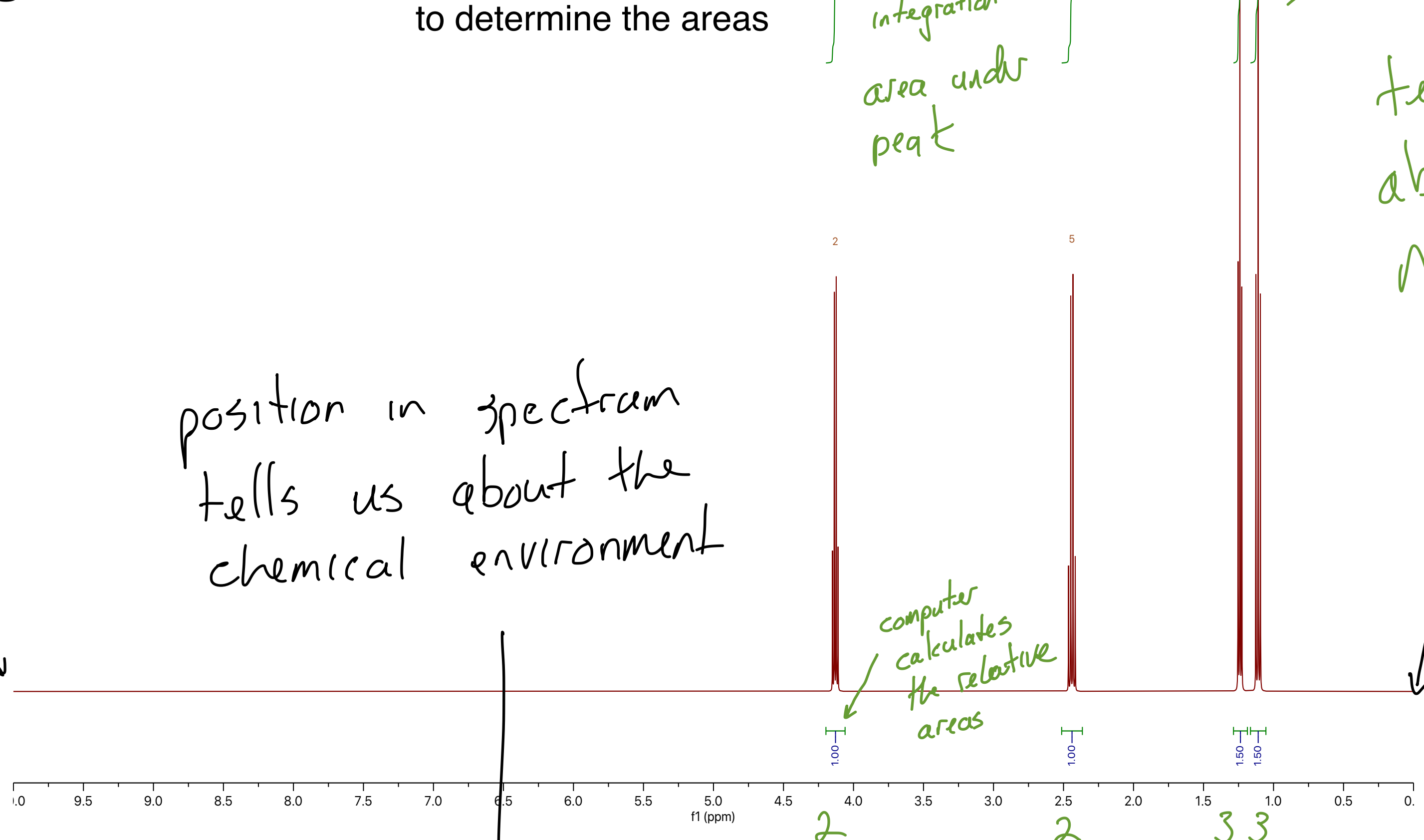


measure the heights to determine the areas →

old school integration
area under peak

multiplicity
shape of peak
tells us about the neighbors

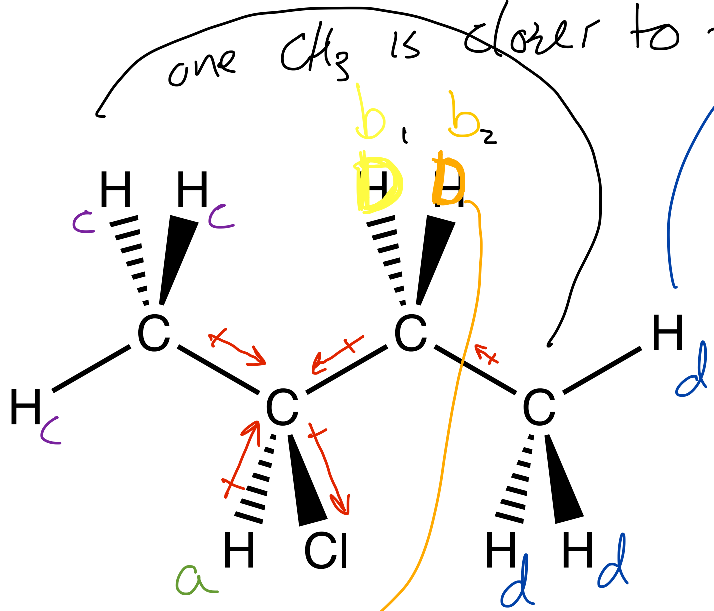
position in spectrum tells us about the chemical environment



# of different types of H atoms 4	Chemical environments of the H atoms	How many of each type of H atom	# of H atom neighbors

What Makes ^{1}H Different

different chemical environment



a is the only H connected to a C with a Cl also present. It is chemically different, which usually means magnetic inequivalency so it resonantes at a different frequency

c all H's attached to same C, get the same products if any of the 3 are replaced chemically equivalent. rotation makes them magnetically equivalent

chemically equivalent and magnetically equivalent due to rotation on C-C bond

d

same? No, replacing 1 H with D gives (2S,3S)-2-chloro-3-deuterobutane and replacing the other H with D gives (2S,3R)-2-chloro-3-deuterobutane

these are diastereomers and they have different properties ∴ these H's are not chemically equivalent

They are diastereotopic. So they are likely to be magnetically inequivalent

$^2J_{(H-H)} = -12.4$ Hz $^1J_{(C-H)} = 125$ Hz

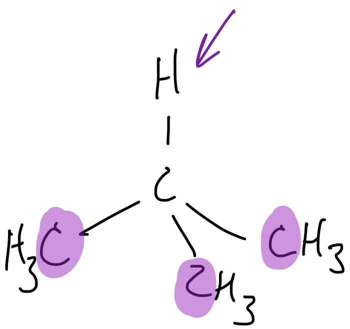
$H-CH_3$ 0.232 ppm   M.J. Lacey   Aust. J. Chem. (1970), 23, 1421.
via National Institute of Advanced Industrial Science and Technology (AIST)

H_3C-CH_3 0.79 ppm — http://u-of-o-nmr-facility.blogspot.com/2012/03/extremely-complicated-1-h-nmr-spectrum.html

$H_3C-CH_2-CH_3$ 1.33, 0.91 — simulation

1.336, 0.899 — N. Sheppard, J.J. Turner Mol. Phys. (1960) 3, 168 via AIST

$^3J_{(H-H)} = 7.4$



1.739, 0.889 — simulation

each time a ^1H is replaced with a more electronegative C atom the resonance frequency of the ^1H's that remain move to higher frequency.