^{13}C NMR Spectroscopy

from chapter ______________ in the recommended text

A. Introduction

B. Fundamental Physics Of NMR (Nuclear Magnetic Resonance)

Nuclear spin

pairing these spins between aligned and counter-aligned states by applying a *radiofrequency*
low energy range of the electromagnetic spectrum, *ie* *low* frequency and *high*

½, and for ^{12}C the nuclear spin is *0*.

high, but that of ^{13}C is *low* (*1.1*

averaged over multiple scans to increase *both these parameters*.

less than those between vibrational states in IR, and *less*
are sensitive to large external magnetic fields

larger the energy gap between nuclear spin states.

the energy gap between the nuclear spin states / Boltzman distributions / both these parameters.

are sensitive to the electron density and proximal NMR active nuclei in the same molecule, hence these nuclei in different parts of the molecule flip when *different*

"*shield* each other

deshielded relative to Chemical Shifts In General

$SiMe_4$.

δ on this scale reflects how much less the frequency is for an NMR active nuclei to flip, or *resonate*,

$$\frac{\text{frequency of 0 on scale} - \text{frequency for nucleus}}{\text{frequency of 0 on scale}}$$

positive.
deshielded
the operating frequency of the machine
200,000,000 Hz.
200 so on
200, *ie* *200* Hz.

on a 250 MHz machine, 1 ppm corresponds to ___250___ Hz in proton NMR spectra
on a 400 MHz machine, 1 ppm corresponds to ___400___ Hz in proton NMR spectra
on an 800 MHz machine, *10 ppm* corresponds to __8000____ Hz in proton NMR spectra

_25_ Hz.
difference of __0.1__ ppm.
___0.1___ ppm.

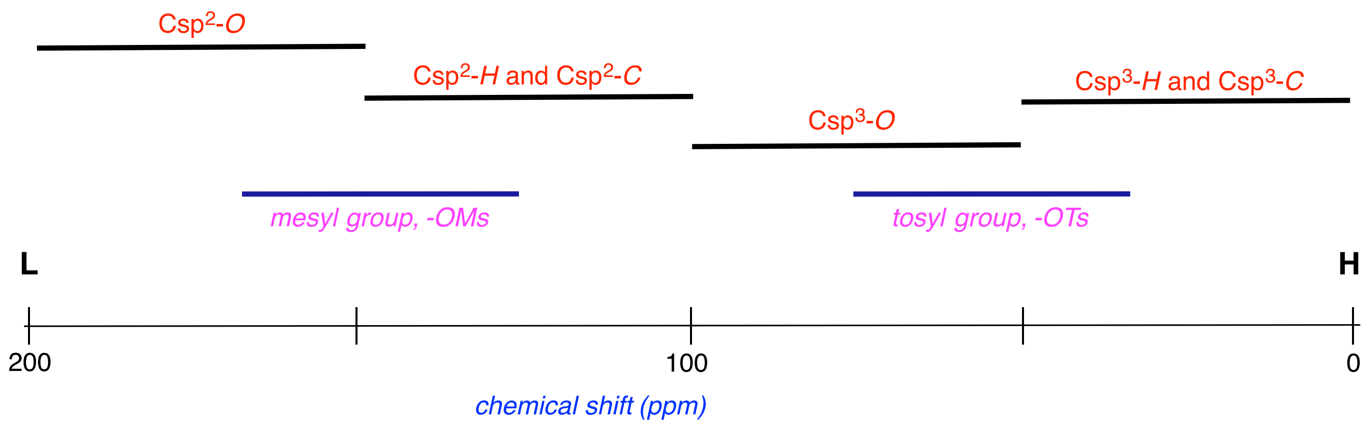
more on a 60 MHz

more on a 100 MHz

less as the operating frequency

C. Chemical Shifts In ^{13}C Spectra

upfield region and corresponds to *shielded*



downfield region and corresponds to *deshielded*

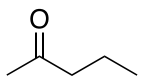
attract electron density tend to *deshield*

deshield

less shielded

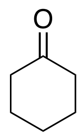
inequivalent except

the same chemical shifts, and inequivalent ones usually resonate at *different* *the same as*



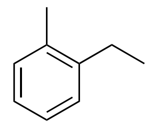
__5__
inequivalent C

number of
resonances (ppm):
0 - 50 __4__
50 - 100 _0__
100 - 150 _0__
above 150 _1__



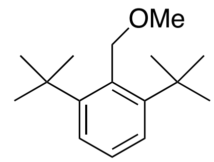
__4__
inequivalent C

number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _0__
above 150 _1__



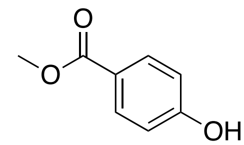
__9__
inequivalent C

number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _6__
above 150 _0__



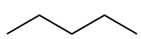
__8__
inequivalent C

number of
resonances (ppm):
0 - 50 _2__
50 - 100 _2__
100 - 150 _4__
above 150 _0__



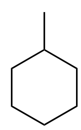
__6__
inequivalent C

number of
resonances (ppm):
*0 - **40** _0__*
***40** - 100 _1__*
100 - 150 _3__
above 150 _2__



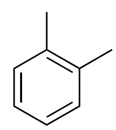
__3__
inequivalent C

number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _0__
*above 150 __0_*



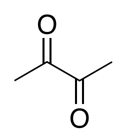
__5__
inequivalent C

number of
resonances (ppm):
0 - 50 _5__
50 - 100 _0__
100 - 150 _0__
above 150 _0__



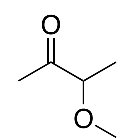
__4__
inequivalent C

number of
resonances (ppm):
0 - 50 _1__
50 - 100 _0__
100 - 150 _3__
above 150 _0__



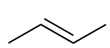
__2__
inequivalent C

number of
resonances (ppm):
0 - 50 _1__
50 - 100 _0__
100 - 150 _0__
above 150 _1__



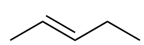
__5__
inequivalent C

number of
resonances (ppm):
0 - 50 _2__
50 - 100 _2__
100 - 150 _0__
above 150 _1__



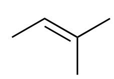
__2__
inequivalent C

number of
resonances (ppm):
0 - 50 _1__
50 - 100 _0__
100 - 150 _1__
above 150 _0__



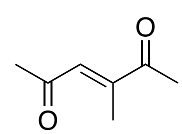
__5__
inequivalent C

number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _2__
above 150 _0__



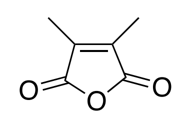
__5__
inequivalent C

number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _2__
above 150 _0__



__7__
inequivalent C

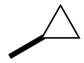
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _2__
above 150 _2__



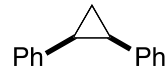
__3__
inequivalent C

number of
resonances (ppm):
0 - 50 _1__
50 - 100 _0__
100 - 150 _1__
above 150 _1__

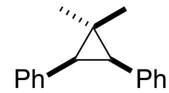
__1__
inequivalent C
number of
resonances (ppm):
0 - 50 _1__
50 - 100 _0__
100 - 150 _0__
above 150 _0__



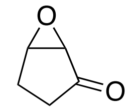
__3__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _0__
above 150 _0__



__6__
inequivalent C
number of
resonances (ppm):
0 - 50 _2__
50 - 100 _0__
100 - 150 _4__
above 150 _0__

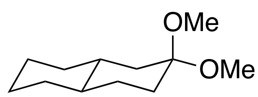


__8__
inequivalent C
number of
resonances (ppm):
0 - 50 _4__
50 - 100 _0__
100 - 150 _4__
above 150 _0__

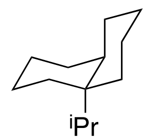


__5__
inequivalent C
number of
resonances (ppm):
0 - **40** _2__
40 - 100 _2__
100 - 150 _0__
above 150 _1__

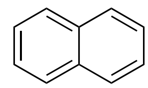
__6__
inequivalent C
number of
resonances (ppm):
0 - 50 _4__
50 - 100 _2__
100 - 150 _0__
above 150 _0__



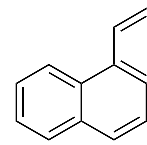
__7__
inequivalent C
number of
resonances (ppm):
0 - 50 _9__
50 - 100 _3__
100 - 150 _0__
above 150 _0__



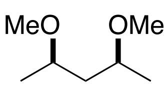
__12__
inequivalent C
number of
resonances (ppm):
0 - 50 _12__
50 - 100 _0__
100 - 150 _0__
above 150 _0__



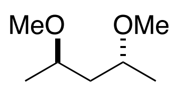
__3__
inequivalent C
number of
resonances (ppm):
0 - 50 _0__
50 - 100 _0__
100 - 150 _3__
above 150 _0__



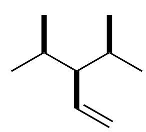
__7__
inequivalent C
number of
resonances (ppm):
0 - 50 _0__
50 - 100 _0__
100 - 150 _7__
above 150 _0__



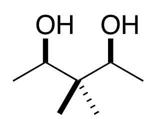
__4__
inequivalent C
number of
resonances (ppm):
0 - 50 _2__
50 - 100 _2__
100 - 150 _0__
above 150 _0__



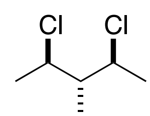
__4__
inequivalent C
number of
resonances (ppm):
0 - 50 _2__
50 - 100 _2__
100 - 150 _0__
above 150 _0__



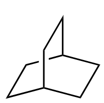
__5__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _2__
above 150 _0__



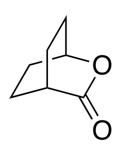
__4__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _1__
100 - 150 _0__
above 150 _0__



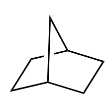
__4__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _1__
100 - 150 _0__
above 150 _0__



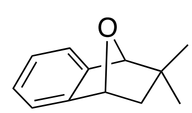
__2__
inequivalent C
number of
resonances (ppm):
0 - 50 _2__
50 - 100 _0__
100 - 150 _0__
above 150 _0__



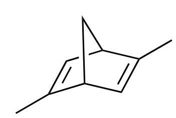
__7__
inequivalent C
number of
resonances (ppm):
0 - 50 _5__
50 - 100 _1__
100 - 150 _0__
above 150 _1__



__3__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _0__
above 150 _0__



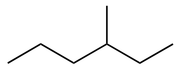
__11__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _2__
100 - 150 _6__
above 150 _0__



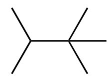
__5__
inequivalent C
number of
resonances (ppm):
0 - 50 _3__
50 - 100 _0__
100 - 150 _2__
above 150 _0__

__6__ ^{13}C resonances.

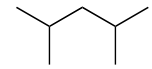
cannot be



7 inequivalent C



4 inequivalent C



3 inequivalent C

D. Coupling In ^{13}C NMR

^{13}CH Spin Systems

The ^{1}H nucleus is

different to

into two peaks of almost equal intensity; this is called a doublet.

The chemical shift of that carbon is exactly at the center of

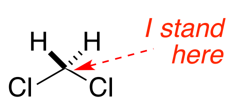
coupling with protons

doublet and a singlet, respectively.

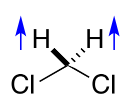
In that experiment it would

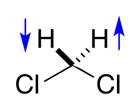
^{13}CH$_2$ Spin Systems

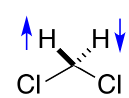
the same

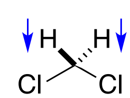


and experience.....









magnetic effect feels same

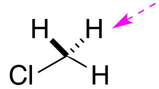
3 different magentic field strengths influence that ^{13}C, ratio 1:2:1

three different magnetic fields and the relative probability is 1:2:1.

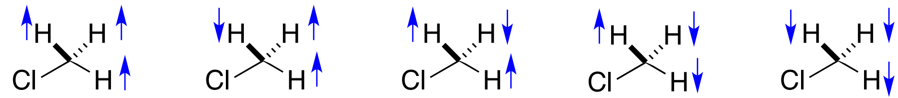
triplet for the carbon and it could

^{13}CH$_3$ Spin Systems

quartet for the carbon and it could



put arrows on all H atoms to indicate spins (as above)



__4__ different magentic field strengths influence that ^{13}C, ratio __1:3:3:1__

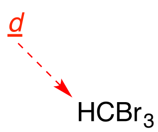
The relative probabilities for finding the spins in *a* or *o* states is *1:3:3:1*.

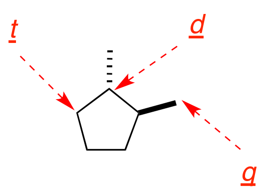
n + 1 peaks.
doing the splitting and not those *being observed*.

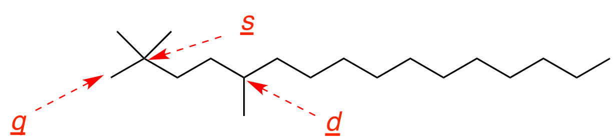
follows Pascal's triangle.

rare and *can* be ignored.

Differentiating CH, CH_2, And CH_3 In ^{13}C Spectra







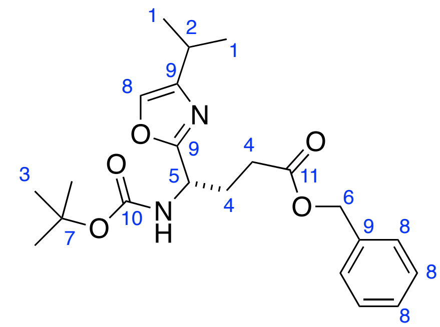
coupling constant and it is expressed in *Hz*.
different on machines operating at different field strengths, so they are *never*

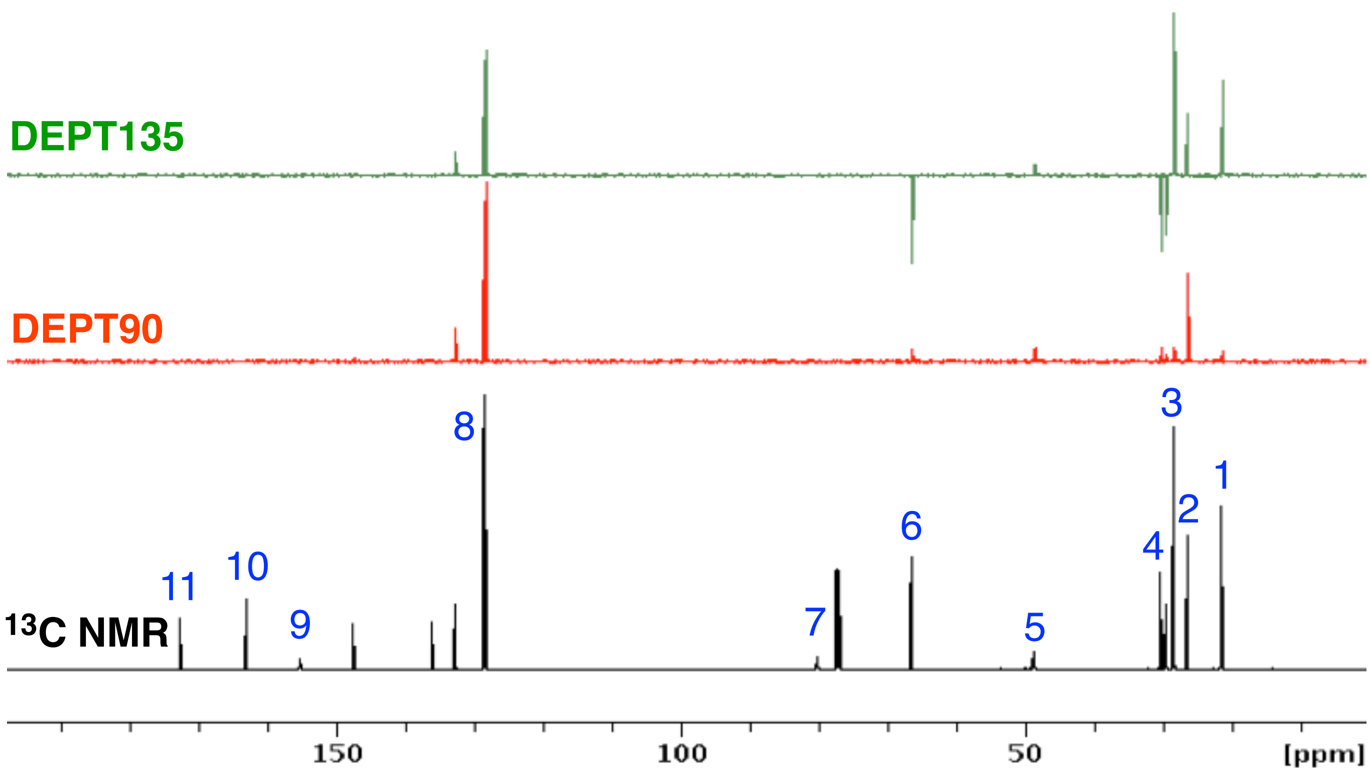
DEPT Spectra To Differentiate Quaternary, Methine-, Methylene-, and Methyl-Carbons

quaternary, *do not*
positive peaks, and resonances for CH_2 carbons *negative*.

CH peaks.

can
more





nearly always shown.

[1]H-NMR signals of the protons attached to them.