

Chapter 13: Spectroscopy

Methods of structure determination

- Nuclear Magnetic Resonances (NMR) Spectroscopy (Sections 13.3-13.19)
- Infrared (IR) Spectroscopy (Sections 13.20-13.22)
- Ultraviolet-visible (UV-Vis) Spectroscopy (Section 13.23)
- Mass (MS) spectrometry (not really spectroscopy) (Section 13.24)

Molecular Spectroscopy: the interaction of electromagnetic radiation (light) with matter (organic compounds). This interaction gives specific structural information.

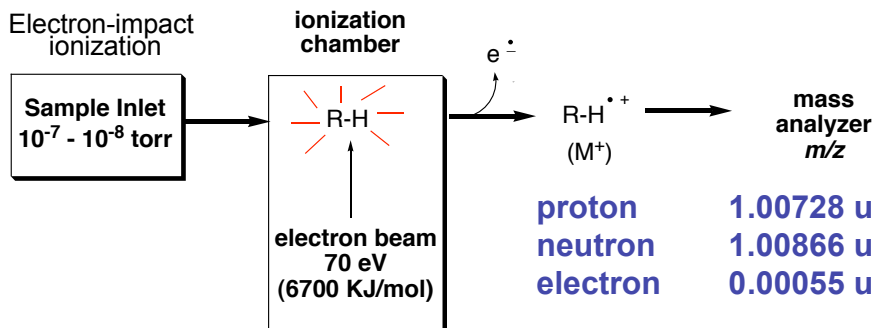
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13.24: Mass Spectrometry:

molecular weight of the sample \longrightarrow formula

The mass spectrometer gives the mass to charge ratio (m/z), therefore the sample (analyte) must be an ion.

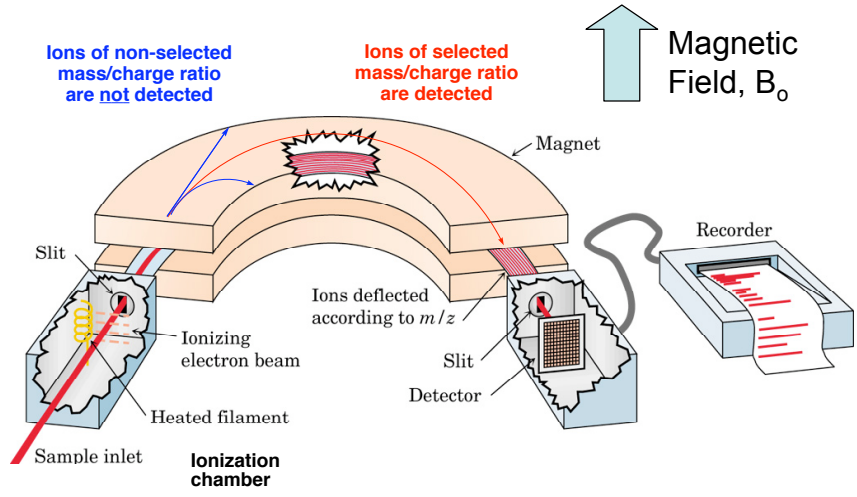
Mass spectrometry is a gas phase technique- the sample must be "vaporized."



2

$$\frac{\text{mass}}{\text{charge}} = \frac{m}{z} = \frac{B^2 r^2}{2V}$$

B = magnetic field strength
 r = radius of the analyzer tube
 V = voltage (accelerator plate)



The Mass Spectrometer

3

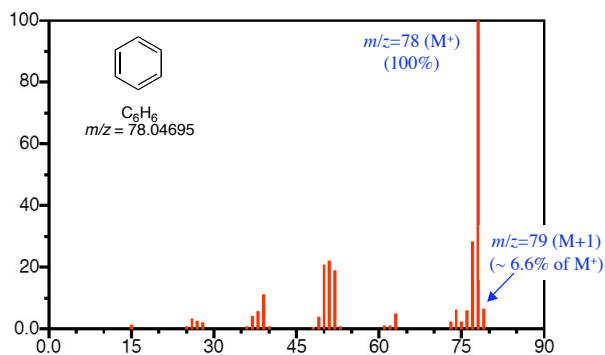
Exact Masses of Common Natural Isotopes

Isotope	mass	natural abundance	Isotope	mass	natural abundance
¹ H	1.00782	99.985	¹⁹ F	18.99840	100.00
² H	2.01410	0.015	³⁵ Cl	34.96885	75.77
¹² C	12.0000	98.892	³⁷ Cl	36.96590	24.23 (32.5%)
¹³ C	13.0033	1.108 (1.11%)	⁷⁹ Br	78.91839	50.69
¹⁴ N	14.00307	99.634	⁸¹ Br	80.91642	49.31 (98%)
¹⁵ N	15.00010	0.366 (0.38%)	¹²⁷ I	126.90447	100.00
¹⁶ O	15.99491	99.763			
¹⁷ O	16.99913	0.037 (0.04%)			
¹⁸ O	17.99916	0.200 (0.20%)			

4

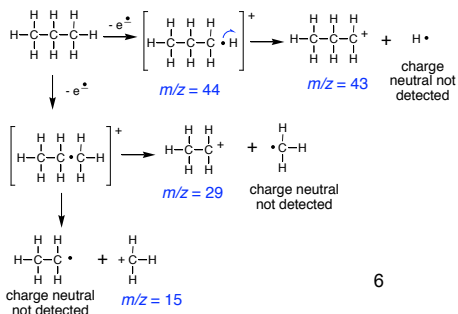
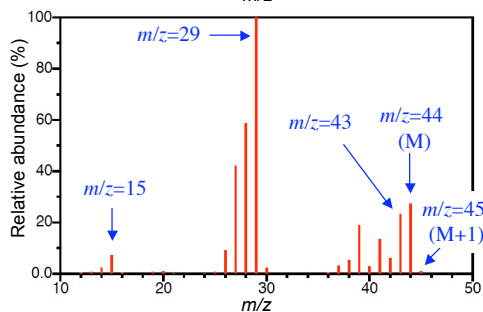
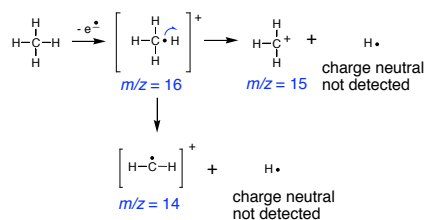
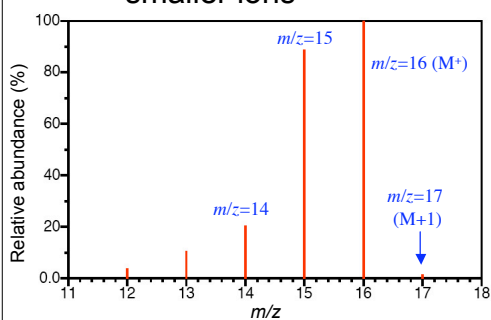
Molecular Ion (parent ion, M) = molecular mass of the analyte;
sample minus an electron

Base peak- largest (most abundant) peak in a mass spectra;
arbitrarily assigned a relative abundance of 100%.

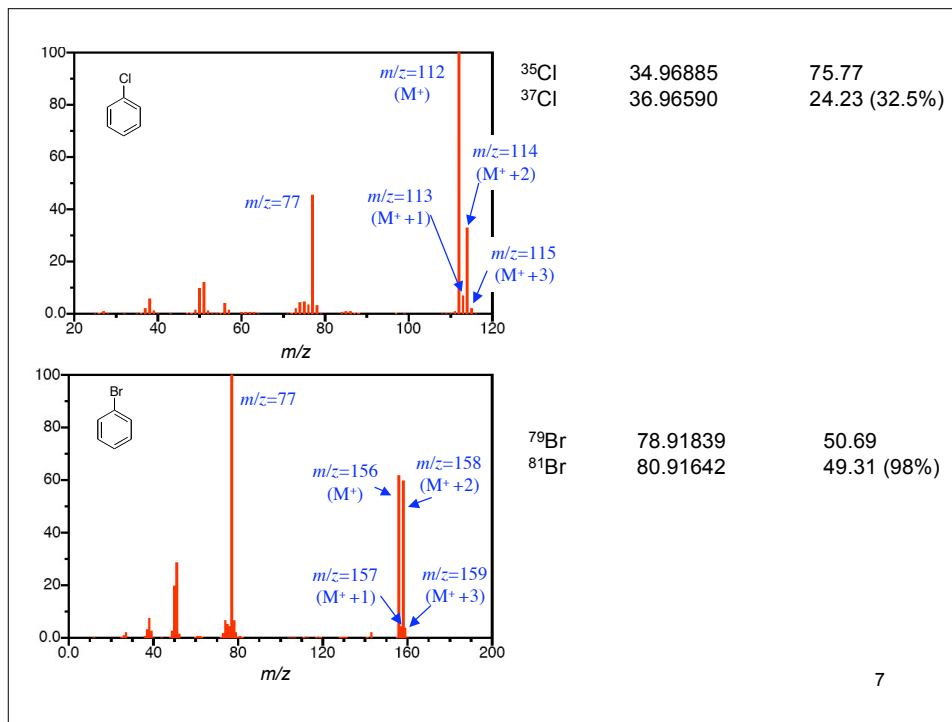


5

The radical cation ($M^{+\bullet}$) is unstable and will fragment into smaller ions



6



Mass spectra can be quite complicated and interpretation difficult.

Some functional groups have characteristic fragmentation

It is difficult to assign an entire structure based only on the mass spectra. However, the mass spectra gives the mass and formula of the sample which is very important information.

To obtain the formula, the molecular ion must be observed.
Soft ionization techniques

Methods have been developed to get large molecules such as polymers and biological macromolecules (proteins, peptides, nucleic acids) into the vapor phase

13.25: Molecular Formula as a Clue to Structure

Nitrogen rule: In general, “small” organic molecules with an odd mass must have an odd number of nitrogens. Organic molecules with an even mass have zero or an even number of nitrogens

If the mass can be determined accurately enough, then the molecular formula can be determined (high-resolution mass spectrometry)

Information can be obtained from the molecular formula:

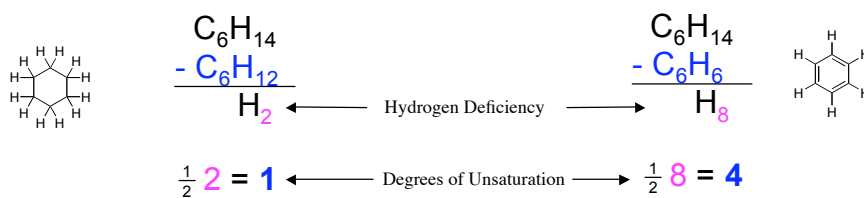
Degrees of unsaturation: the number of rings and/or π -bonds in a molecule (Index of Hydrogen Deficiency)

9

Degrees of unsaturation

saturated hydrocarbon	C_nH_{2n+2}
cycloalkane (1 ring)	C_nH_{2n}
alkene (1 π -bond)	C_nH_{2n}
alkyne (2 π -bonds)	C_nH_{2n-2}

For each ring or π -bond, -2H from the formula of the saturated alkane



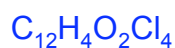
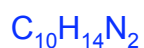
10

Correction for other elements:

For Group VII elements (halogens): subtract 1H from the H-deficiency for each halogen,

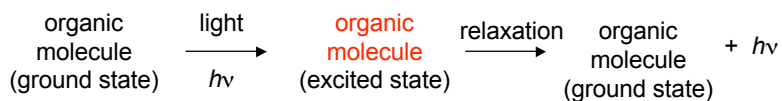
For Group VI elements (O and S): No correction is needed

For Group V elements (N and P): add 1H to the H-deficiency for each N or P

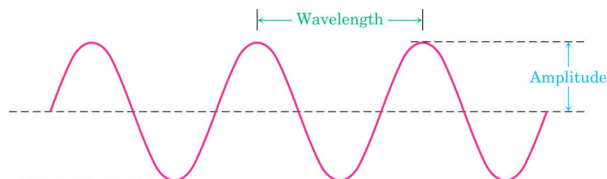


11

13.1: Principles of molecular spectroscopy: Electromagnetic radiation



Electromagnetic radiation has the properties of a particle (photon) *and* a wave.



λ = distance of one wave

ν = frequency: waves per unit time (sec^{-1} , Hz)

c = speed of light ($3.0 \times 10^8 \text{ m} \cdot \text{sec}^{-1}$)

h = Planck's constant ($6.63 \times 10^{-34} \text{ J} \cdot \text{sec}$)

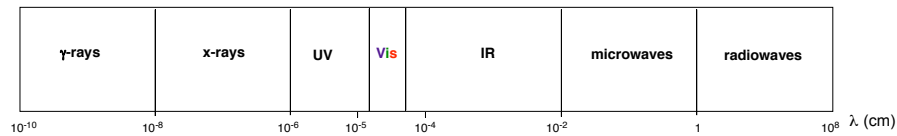
12

Quantum: the energy of a photon

$$E = h\nu \quad \nu = \frac{c}{\lambda}$$

$$E = \frac{h \cdot c}{\lambda}$$

$$E \propto \nu \quad E \propto \lambda^{-1} \quad \nu \propto \lambda^{-1}$$

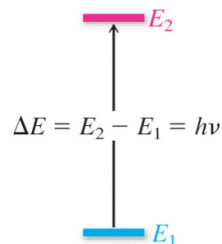


short ←———— Wavelength (λ) —————→ long
 high ←———— Frequency (ν) —————→ low
 high ←———— Energy (E) —————→ low

13

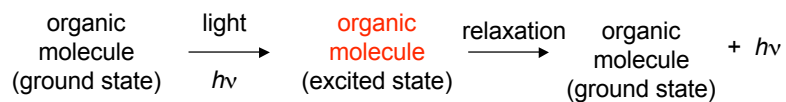
13.1: Principles of molecular spectroscopy: Quantized Energy Levels

molecules have discrete energy levels
(no continuum between levels)



A molecule absorbs electromagnetic radiation when the energy of photon corresponds to the difference in energy between two states

14



UV-Vis: valance electron transitions

- gives information about π -bonds and conjugated systems

Infrared: molecular vibrations (stretches, bends)

- identify functional groups

Radiowaves: nuclear spin in a magnetic field (NMR)

- gives a map of the H and C framework

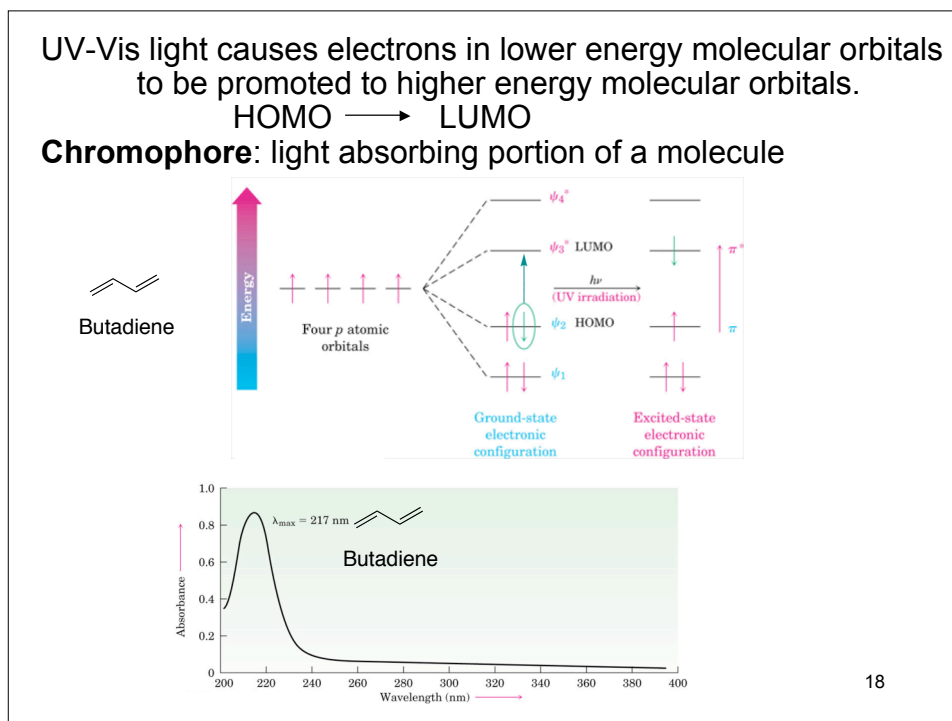
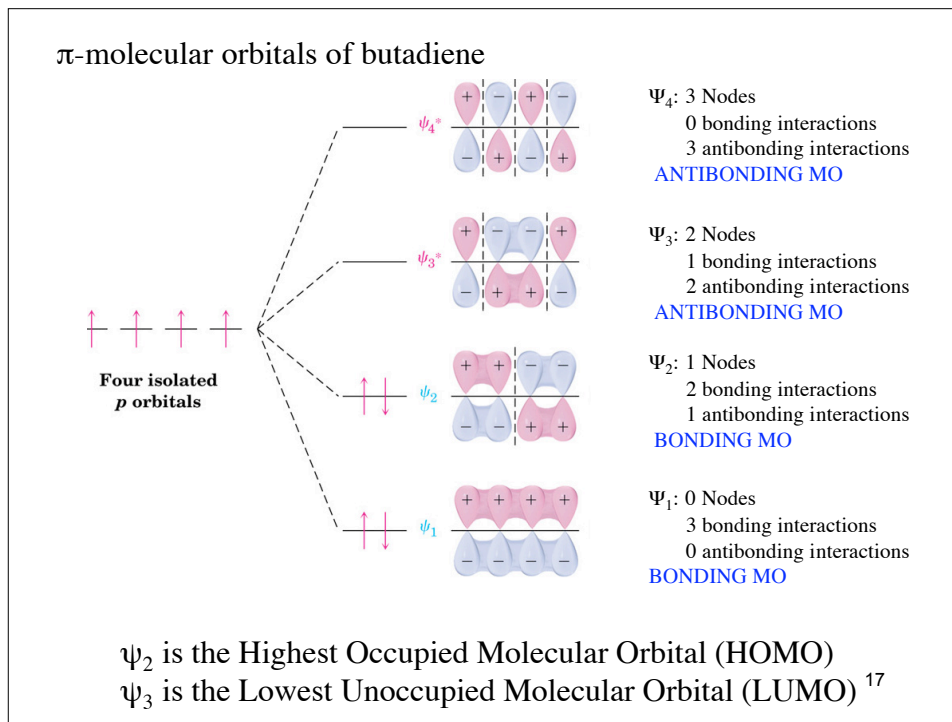
15

13.23 Ultraviolet-Visible (UV-Vis) Spectroscopy

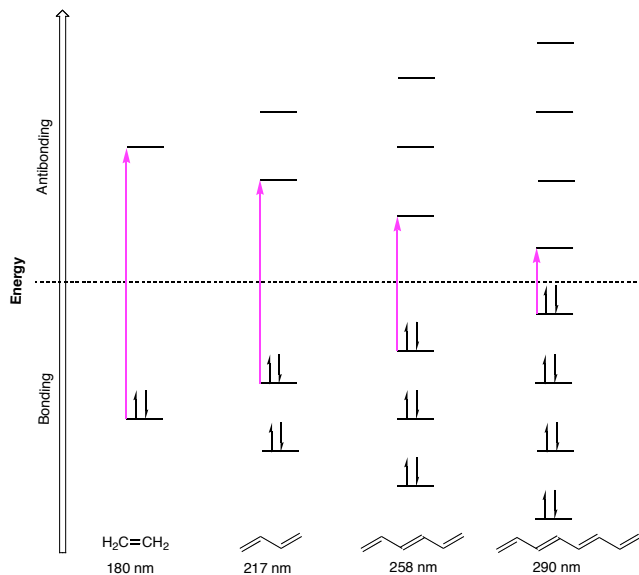


Recall bonding of a π -bond from Chapter 10.16

16

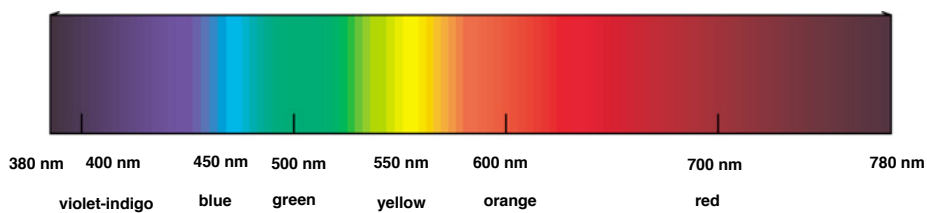


Molecular orbitals of conjugated polyenes



19

Molecules with extended conjugation move toward the visible region



Color of absorbed light

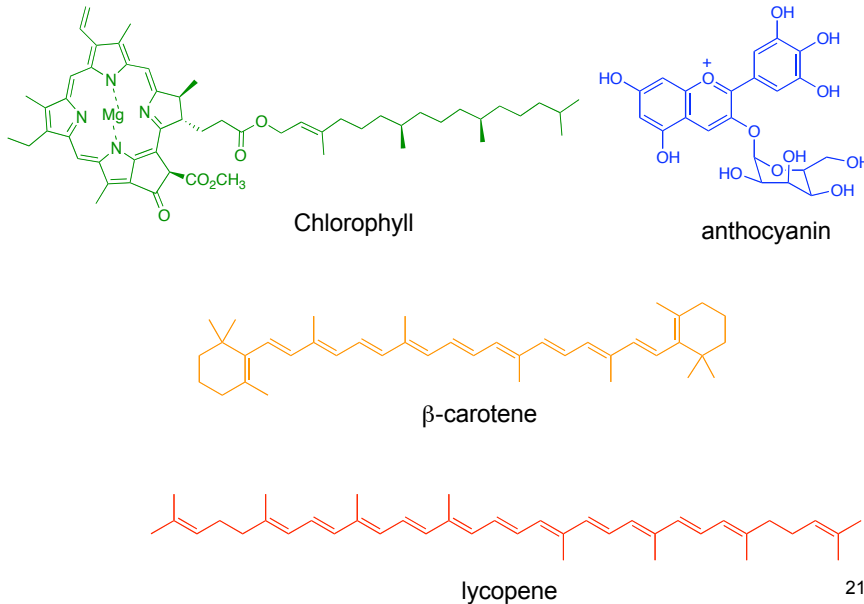
λ

Color observed

violet	400 nm	yellow
blue	450	orange
blue-green	500	red
yellow-green	530	red-violet
yellow	550	violet
orange	600	blue-green
red	700	green

20

Many natural pigments have conjugated systems



21

Chromophore: light absorbing portion of a molecule

Beer's Law: There is a linear relationship between absorbance and concentration

$$A = \epsilon c l$$

A = absorbance

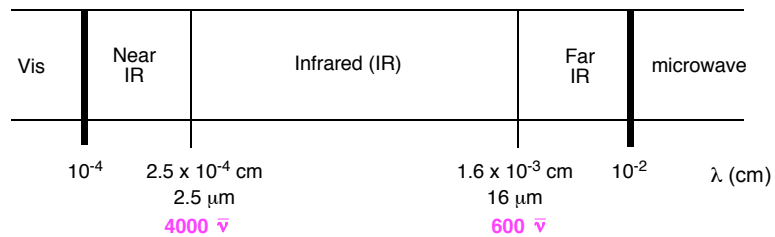
c = concentration (M, mol/L)

l = sample path length (cm)

ϵ = molar absorptivity (extinction coefficient)
a proportionality constant for a specific absorbance of a substance

22

13.20: Introduction to Infrared Spectroscopy

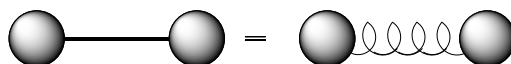


$$E \propto \frac{1}{\lambda}$$

λ is expressed as $\bar{\nu}$ (wavenumber), reciprocal cm (cm⁻¹)

$$\bar{\nu} = \frac{1}{\lambda} \quad \text{therefore} \quad E \propto \bar{\nu}$$

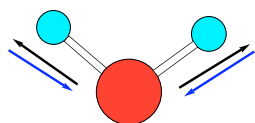
IR radiation causes changes in a molecular vibrations



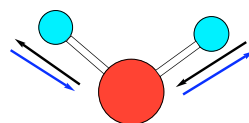
23

Stretch: change in bond length

<http://www2.chem.ucalgary.ca/Flash/photon.html>

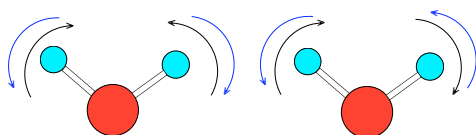


Symmetric stretch



Antisymmetric stretch

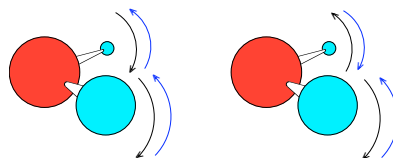
Bend: change in bond angle



scissoring

rocking

in-plane bend



wagging

twisting

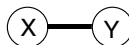
out-of-plane bend

Animation of bond stretches and bends:

<http://wetcbe.cmbi.ru.nl//organic/vibr/methamjm.html>

24

Bond Stretch:
Hooke's Law



$$\bar{\nu} = \frac{1}{2 \pi c} \left[\frac{f}{\left(\frac{m_x m_y}{m_x + m_y} \right)} \right]^{\frac{1}{2}}$$

$\bar{\nu}$ = vibrational frequency

c = speed of light

m_x = mass of X

m_y = mass of Y

$$\left(\frac{m_x m_y}{m_x + m_y} \right) = \text{reduced mass } (\mu)$$

f = spring constant; type of bond between X and Y (single, double or triple)

$$E \propto \bar{\nu} \propto f$$

Hooke's law simulation:

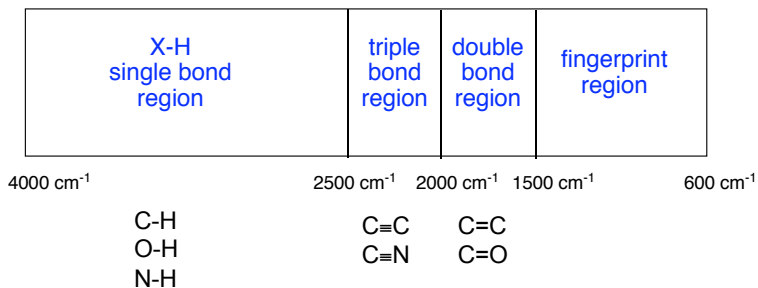
<http://www2.chem.ucalgary.ca/Flash/hooke.html>

25

Interpretation of an Infrared Spectra:

organic molecules contain many atoms. As a result, there are many stretching and bending modes- IR spectra have many absorption bands

Four distinct regions of an IR spectra



26

Fingerprint region (600 - 1500 cm^{-1})- low energy single bond stretching and bending modes. The fingerprint region is unique for any given organic compound. However, there are few diagnostic absorptions.

Double-bond regions (1500 - 2000 cm^{-1})

C=C 1620 - 1680 cm^{-1}

C=O 1680 - 1790 cm^{-1}

Triple-bond region: (2000 - 2500 cm^{-1})

C \equiv C 2100 - 2200 cm^{-1} (weak, often not observed)

C \equiv N 2240 - 2280 cm^{-1}

X-H Single-bond region (2500 - 4000 cm^{-1})

O-H 3200 - 3600 cm^{-1} (broad)

CO-OH 2500-3600 cm^{-1} (very broad)

N-H 3350 - 3500 cm^{-1}

C-H 2800 - 3300 cm^{-1}

sp³ -C-H 2850 - 2950 cm^{-1}

sp² =C-H 3000 - 3100 cm^{-1}

sp \equiv C-H 3310 - 3320 cm^{-1}

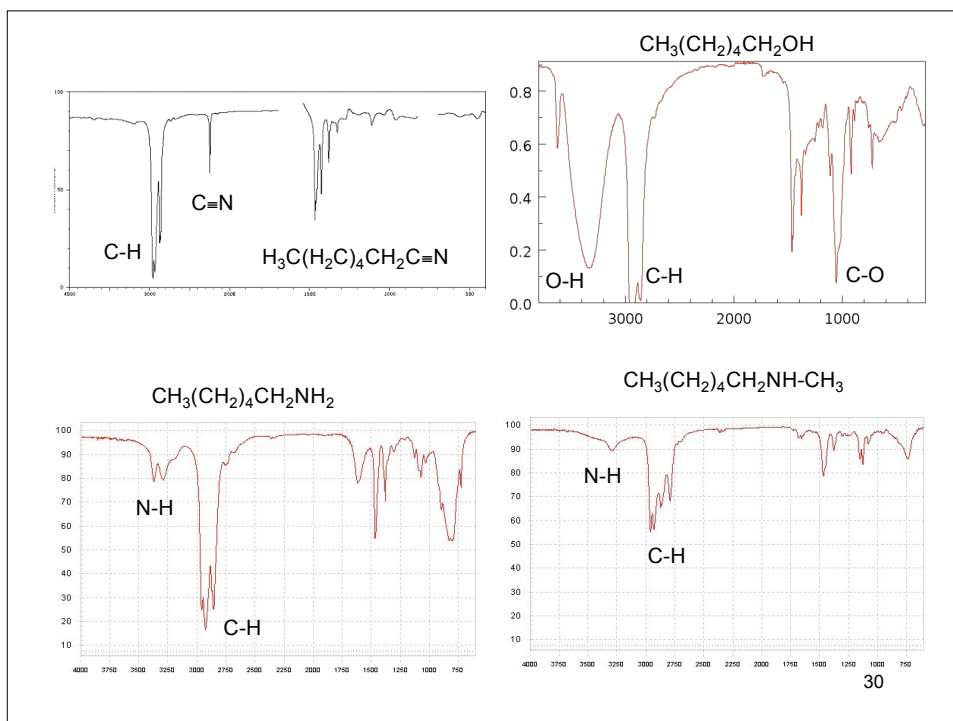
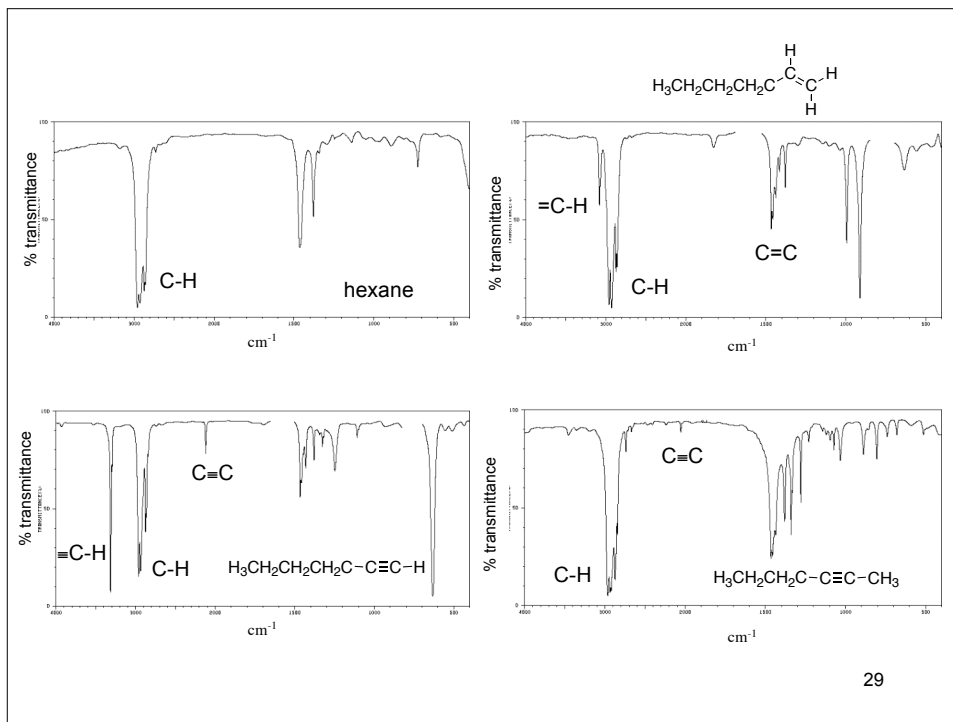
27

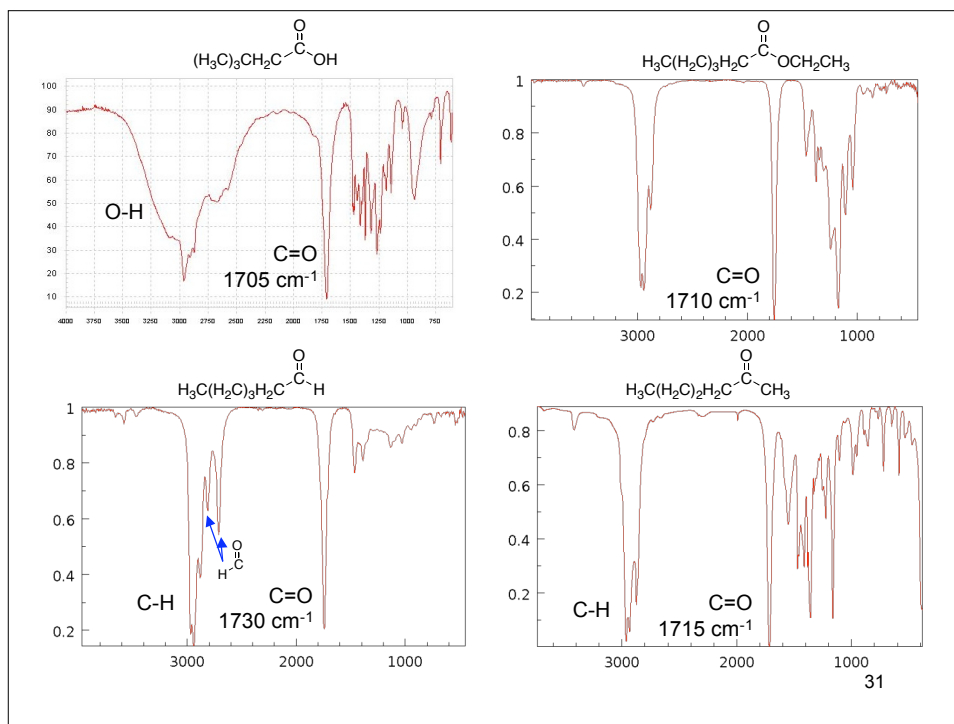
13.22 Characteristic Absorption Frequencies

Table 13.4, p. 554

Alkenes		
	=C-H	3020 - 3100 cm^{-1}
	C=C	1640 - 1680 cm^{-1}
		medium - strong
		medium
Aromatic		
	=C-H	3030 cm^{-1}
	C=C	1450 - 1600 cm^{-1}
		strong
		strong
Alkynes		
	\equiv C-H	3300 cm^{-1}
	C \equiv C	2100-2260 cm^{-1}
		strong
		weak - medium
Alcohols		
	C-O	1050 - 1150 cm^{-1}
	O-H	3400 - 3600 cm^{-1}
		strong
		strong and broad
Amines		
	C-N	1030 - 1230 cm^{-1}
	N-H	3300 - 3500 cm^{-1}
		medium
		medium
Carbonyl		
	C=O	1670 - 1780 cm^{-1}
		strong
Carboxylic acids		
	O-H	2500 - 3500 cm^{-1}
		strong and very broad
Nitrile		
	C \equiv N	2240 - 2280 cm^{-1}
		weak-medium

28





Typical IR Absorptions for Functional Groups

4000	3000	2000	1000	600
X-H Region (2500-4000 cm ⁻¹)		Triple Bond Region (2000-2500)	Double Bond Region (1500-2000)	
C-H O-H N-H		C≡C C≡N	C=C C=O C=N	
Fingerprint Region (600-1500 cm ⁻¹) difficult to interpret				

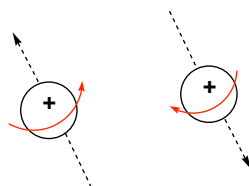
Functional Group	cm ⁻¹	Functional Group	cm ⁻¹
Alkanes, Alkyl groups		Amines	
C-H	2850-2960	N-H	3300-3500
Alkenes		Amide	
=C-H	3020-3150	N-H	3180-3350
C=C	1600-1700	Carbonyl Group	
Alkynes		C=O	1650-1780
=C-H	3300	Carboxylic Acids	
C=C	2100-2200	O-H	2500-3100
Alkyl Halides		Nitriles	
C-Cl	600-800	C=N	2210-2260
C-Br	500-600	Nitro Group	
C-I	500	-NO ₂	1540
Alcohols			
O-H	3400-3650		
C-O	1050-1150		
Aromatics			
=C-H	3030		
	1600, 1500		

32

13.3: Introduction to ^1H NMR

direct observation of the H's of a molecules

Nuclei are positively charged and spin on an axis; they create a tiny magnetic field



Not all nuclei are suitable for NMR.

^1H and ^{13}C are the most important NMR active nuclei in organic chemistry

Natural Abundance

^1H	99.9%	^{13}C	1.1%
		^{12}C	98.9% (not NMR active)

33

- (a) Normally the nuclear magnetic fields are randomly oriented
(b) When placed in an external magnetic field (B_0), the nuclear magnetic field will either aligned with (lower energy) or oppose (higher energy) the external magnetic field

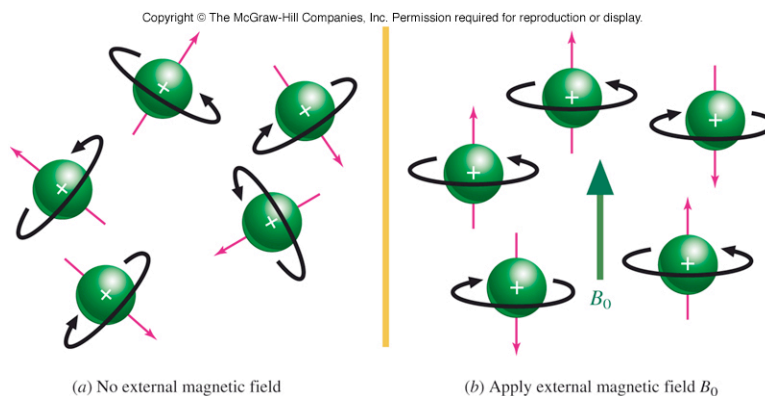
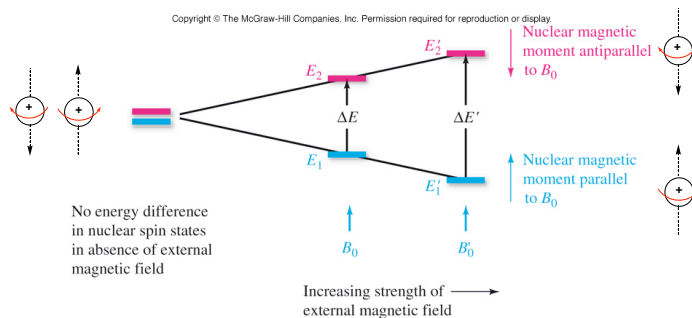


Fig 13.3, p. 520

34

The energy difference between aligned and opposed to the external magnetic field (B_0) is generally small and is dependant upon B_0 . Applied EM radiation (radio waves) causes the spin to flip and the nuclei are said to be in **resonance** with B_0 .



$$\Delta E = h \nu \quad \Delta E = \frac{\gamma B_0 h}{2\pi}$$

B_0 = external magnetic field strength
 γ = gyromagnetic ratio
 $^1\text{H} = 26,752$
 $^{13}\text{C} = 6.7$

Note that $\frac{h}{2\pi}$ is a constant and is sometimes denoted as \hbar 35

NMR Active Nuclei: nuclear spin quantum number (I)
 atomic mass and atomic number

Number of spin states = $2I + 1$ (number of possible energy levels)

Even mass nuclei that have even number of neutrons have $I = 0$
 (NMR inactive)

Even mass nuclei that have odd number of neutrons have an
 integer spin quantum number ($I = 1, 2, 3,$ etc)

Odd mass nuclei have half-integer spin quantum number
 ($I = 1/2, 3/2, 5/2,$ etc)

$I = 1/2$: ^1H , ^{13}C , ^{19}F , ^{31}P

$I = 1$: ^2H , ^{14}N

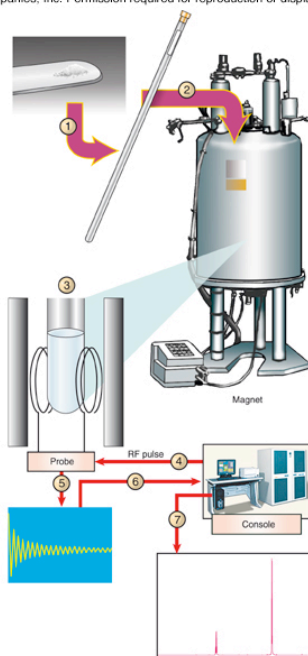
$I = 3/2$: ^{15}N

$I = 0$: ^{12}C , ^{16}O

36

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1. Dissolve sample in CDCl_3 and place in NMR tube.
2. Insert NMR tube into vertical cavity (bore) of the magnet.
3. Bore of magnet contains a probe that acts as a transmitter of radiofrequency (RF) pulses and receiver of signals from the sample. The transmitter is housed in a console along with other electronic equipment.
4. A short ($5 \mu\text{s}$), intense RF pulse is sent from the RF transmitter in the console to the probe. Absorption of RF energy tips the magnetic vector of the nuclei in the sample.
5. The magnetic field associated with the new orientation of the nuclei returns (relaxes) to the original state. Nuclei relax rapidly but at different rates that depend on their chemical environment. As the magnetic field changes, it generates an electrical impulse that is transmitted from the probe to a receiver in the console as a "free induction decay".
6. The pulse-relax sequence is repeated many times and the free-induction decay data stored in a computer in the console.
7. A mathematical operation called a Fourier transform carried out by the computer converts the amplitude-versus-time data of the free-induction decay to amplitude versus frequency and displays the resulting spectrum on the screen or prints it.



Continuous wave
(CW) NMR
Pulsed (FT) NMR

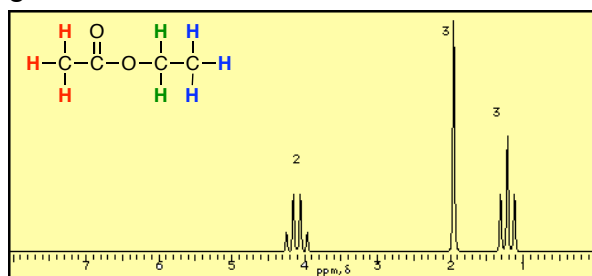
37

13.4: Nuclear Shielding and ^1H Chemical Shift

Different nuclei absorb EM radiation at different wavelengths
(energy required to bring about resonance)

Nuclei of a given type, will resonate at different energies
depending on their chemical and electronic environment.

The position (*chemical shift*, δ) and pattern (*splitting* or *multiplicity*)
of the NMR signals gives important information about the
chemical environment of the nuclei. The *integration* of the
signal is proportional to the number of nuclei giving rise to
that signal

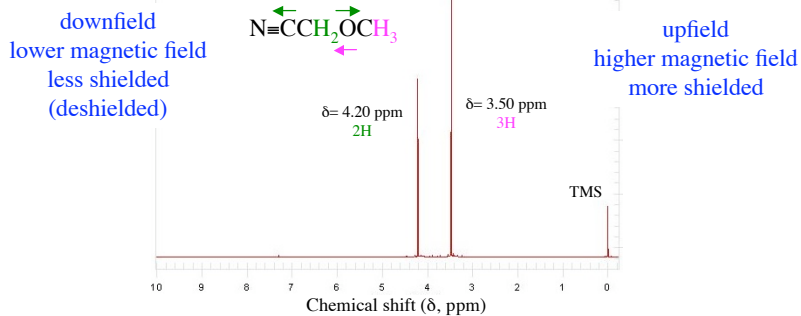
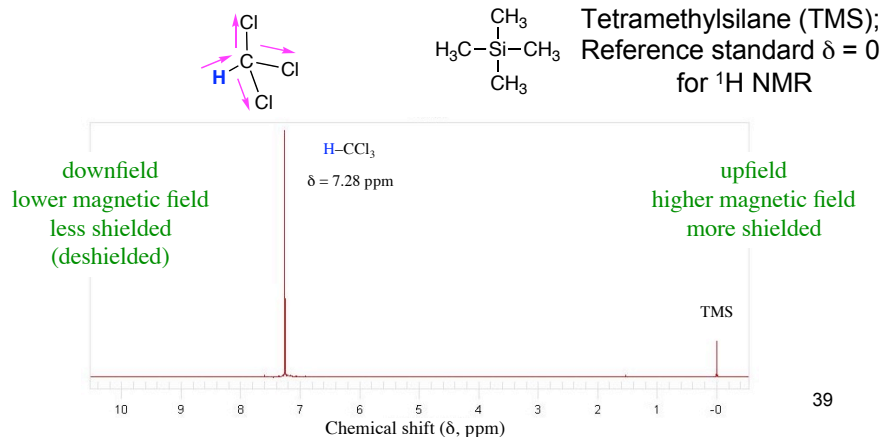


38

Chemical shift: the exact field strength (in ppm) that a nuclei comes into resonance relative to a reference standard (TMS)

Electron clouds “shield” nuclei from the external magnetic field causing them to resonate at slightly higher energy

Shielding: influence of neighboring functional groups on the electronic structure around a nuclei and consequently the chemical shift of their resonance.



Vertical scale= intensity of the signal

Horizontal scale= chemical shift (δ), dependent upon the field strength of the external magnetic field; for ^1H , δ is usually from 1-10 ppm

$$\delta = \frac{\nu - \nu_{\text{TMS}}}{\nu_0} = \frac{\text{chemical shift in Hz}}{\text{operating frequency in MHz}}$$

14,100 gauss: 60 MHz for ^1H (60 million hertz) ppm = 60 Hz
 15 MHz for ^{13}C

140,000 gauss: 600 MHz for ^1H ppm = 600 Hz
 150 MHz for ^{13}C

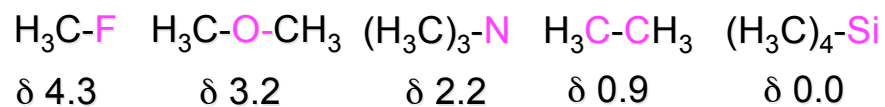
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13.5: Effect of Molecular Structure on ^1H Chemical Shift

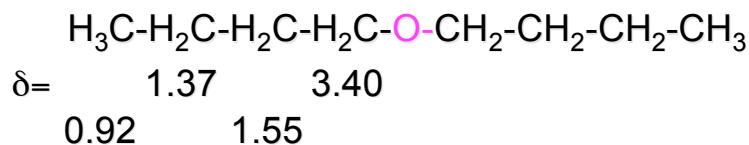
Electronegative substituents deshield nearby protons

less shielded

more shielded

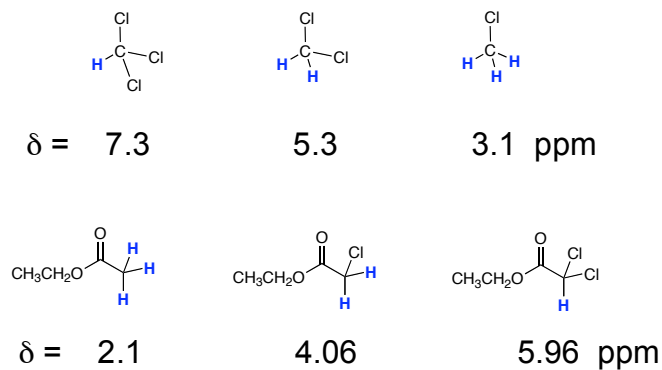


The deshielding effect of a group drops off quickly with distance
(number of bonds between the substituent and the proton)



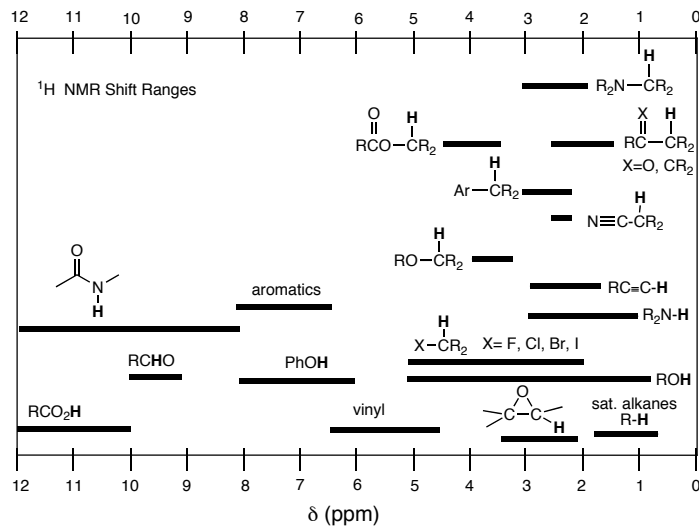
41

The influence of neighboring groups (deshielding) on ^1H chemical shifts is cumulative



42

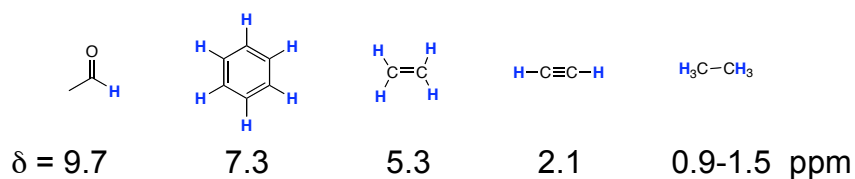
Typical ^1H NMR chemical shifts ranges; additional substitution can move the resonances out of the range



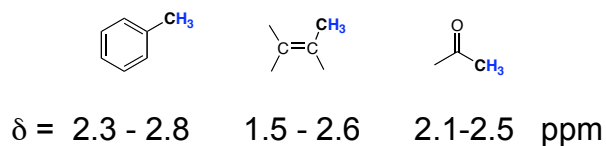
also see Table 13.1 (p. 526)

43

Protons attached to sp^2 and sp hybridize carbons are deshielded relative to protons attached to sp^3 hybridized carbons



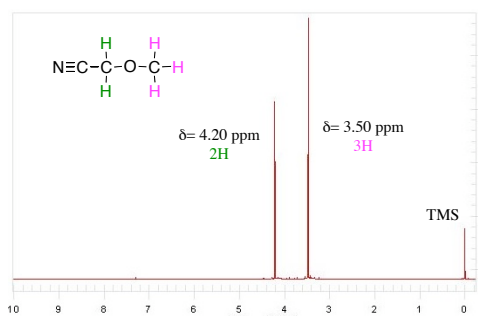
Please read about ring current effects of π -bonds
(Figs. 13.8-13.10, p. 527-9)



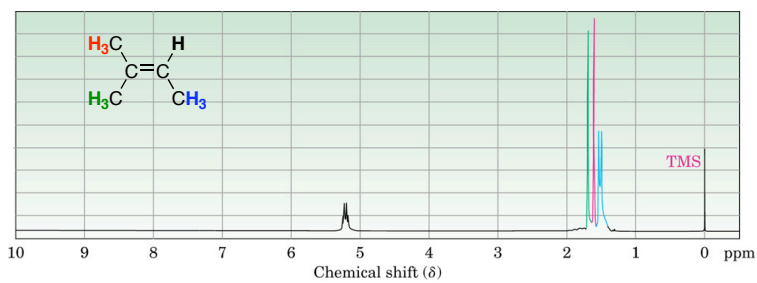
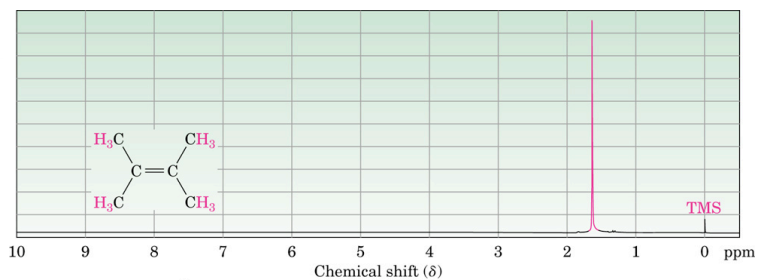
44

13.6: Interpreting ^1H NMR Spectra

Equivalence (chemical-shift equivalence): chemically and magnetically equivalent nuclei resonate at the same energy and give a single signal or pattern



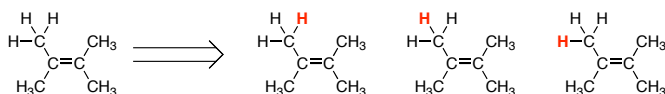
45



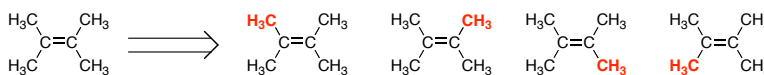
46

Test of Equivalence:

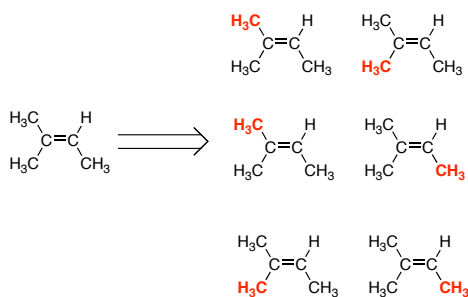
1. Do a mental substitution of the nuclei you are testing with an arbitrary label
 2. Ask what is the relationship of the compounds with the arbitrary label
 3. If the labeled compounds are identical (or enantiomers), then the original nuclei are chemically equivalent and do not normally give rise to a separate resonance in the NMR spectra
- If the labeled compounds are not identical (and not enantiomers), then the original nuclei are not chemically equivalent and can give rise to different resonances in the NMR spectra



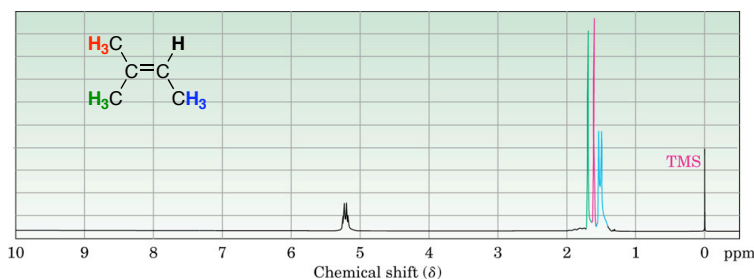
Identical, so the protons are equivalent



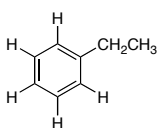
Identical, so the methyl groups are equivalent ⁴⁷



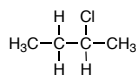
These are geometric isomers (not identical and not enantiomers). The three methyl groups are therefore not chemically equivalent and *can* give rise to different resonances



48



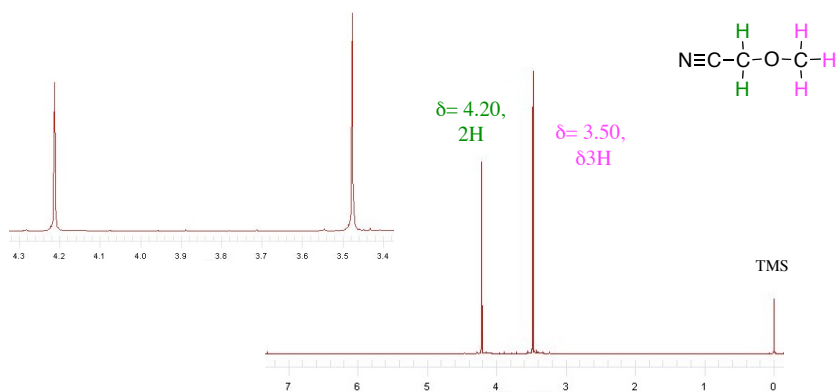
49



Homotopic: equivalent
Enantiotopic: equivalent
Diastereotopic: non-equivalent

50

Integration of ^1H NMR resonances: The area under an NMR resonance is proportional to the number of equivalent nuclei that give rise to that resonance.



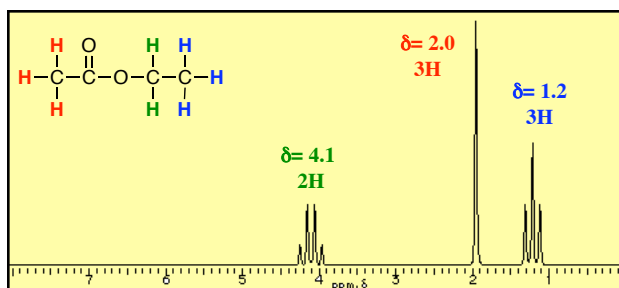
The relative area under the resonances at $\delta = 4.20$ and 3.50 is 2:3

51

13.7: Spin-spin splitting in ^1H NMR spectroscopy

protons on adjacent carbons will interact and “split” each others resonances into multiple peaks (multiplets)

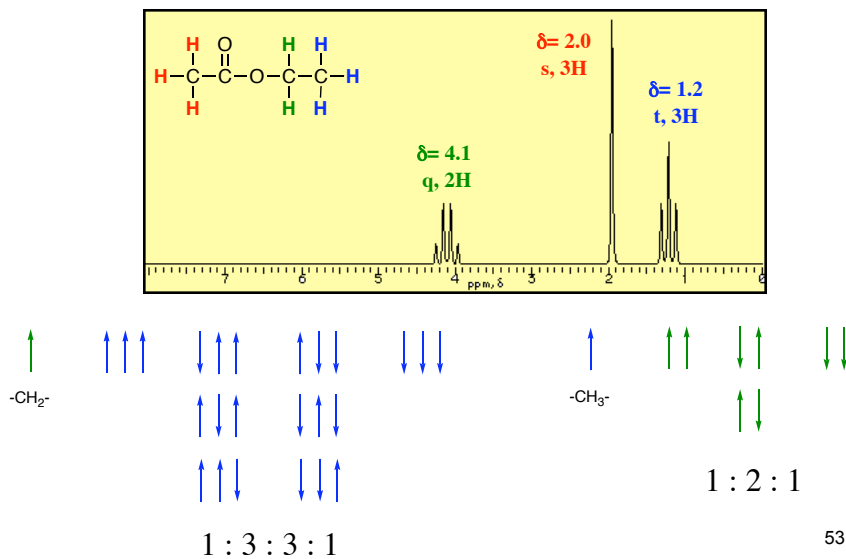
n + 1 rule: equivalent protons that have n equivalent protons on the adjacent carbon will be “split” into n + 1 peaks.



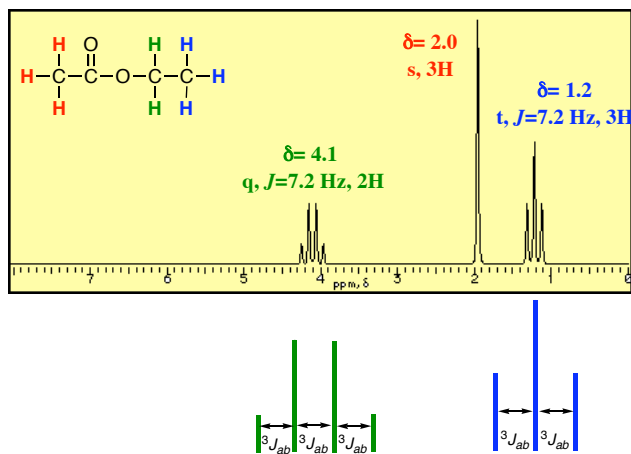
Resonances always split each other. The resonance at $\delta = 4.1$ splits the resonance at $\delta = 1.2$; therefore, the resonance at $\delta = 1.2$ must split the resonance at $\delta = 4.2$.

52

The *multiplicity* is defined by the number of peaks and the pattern (see Table 13.2 for common multiplicities patterns and relative intensities)

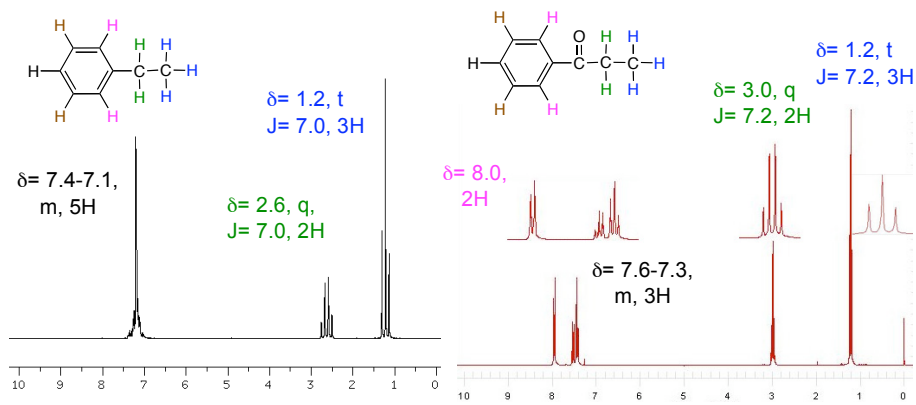


The resonance of a proton with n equivalent protons on the adjacent carbon will be “split” into $n + 1$ peaks with a *coupling constant* J .
Coupling constant: distance between peaks of a split pattern; J is expressed in Hz. Protons coupled to each other have the same coupling constant J .



13.8: Splitting Patterns: The Ethyl Group

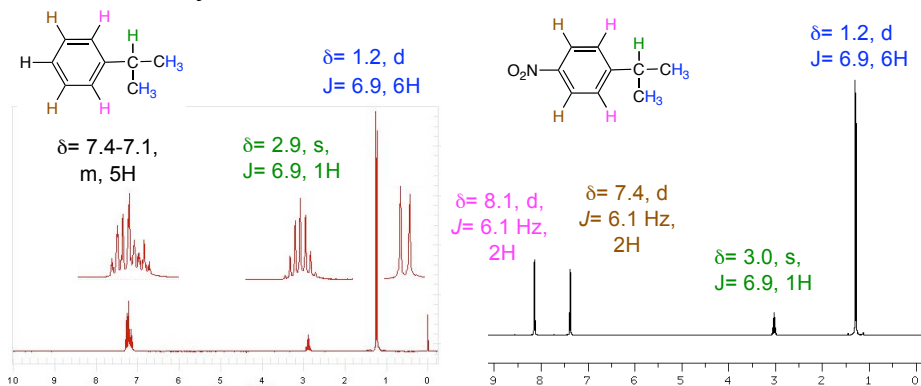
Two equivalent protons on an adjacent carbon will split a proton a **triplet** (t), three peaks of 1:2:1 relative intensity
 Three equivalent protons on an adjacent carbon will split a proton into a **quartet** (q), four peaks of 1:3:3:1 relative intensity



55

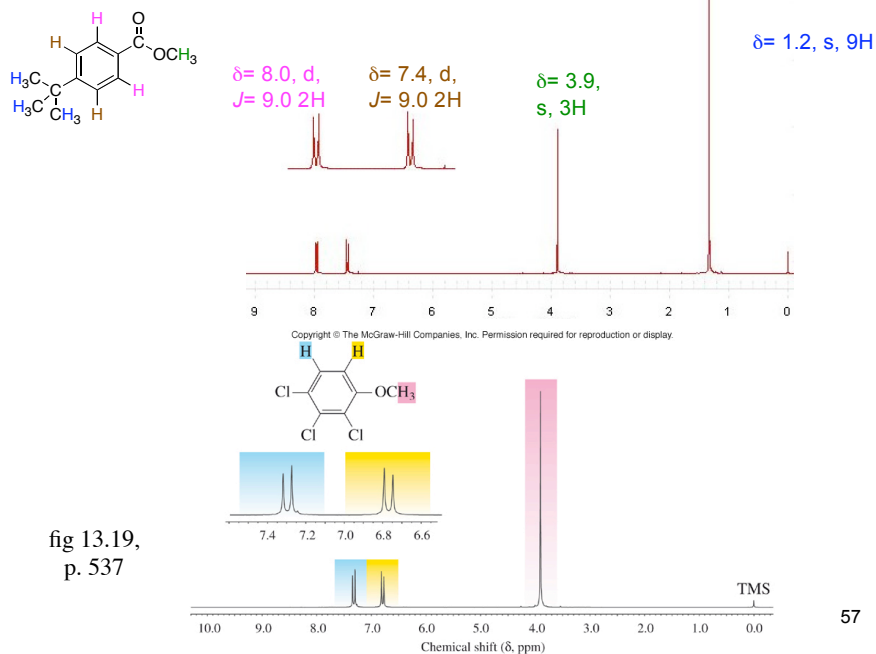
13.8: Splitting Patterns: The Isopropyl Group

One proton on an adjacent carbon will split a proton into a **doublet** (d), two peaks of 1:1 relative intensity
 Six equivalent protons on an adjacent carbon will split a proton into a **septet** (s), seven peaks of 1:6:15:20:15:6:1 relative intensity



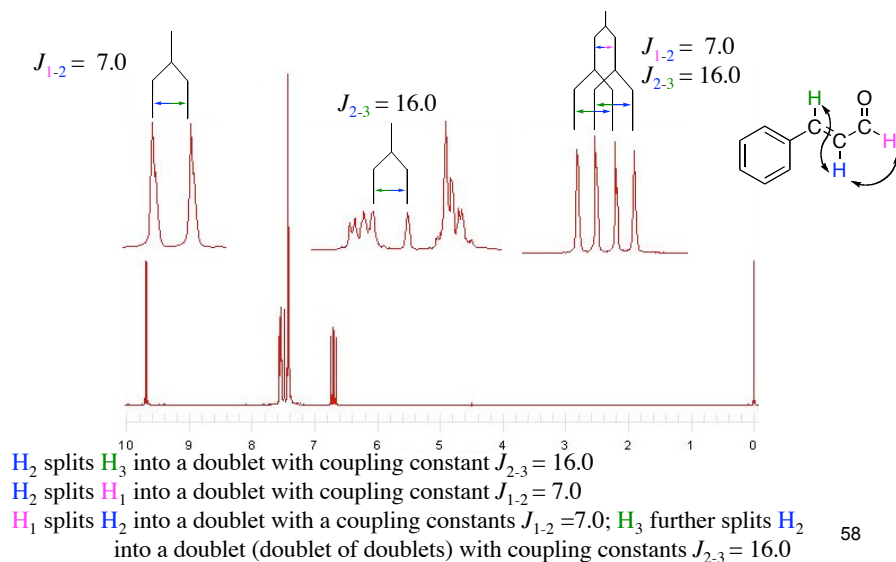
56

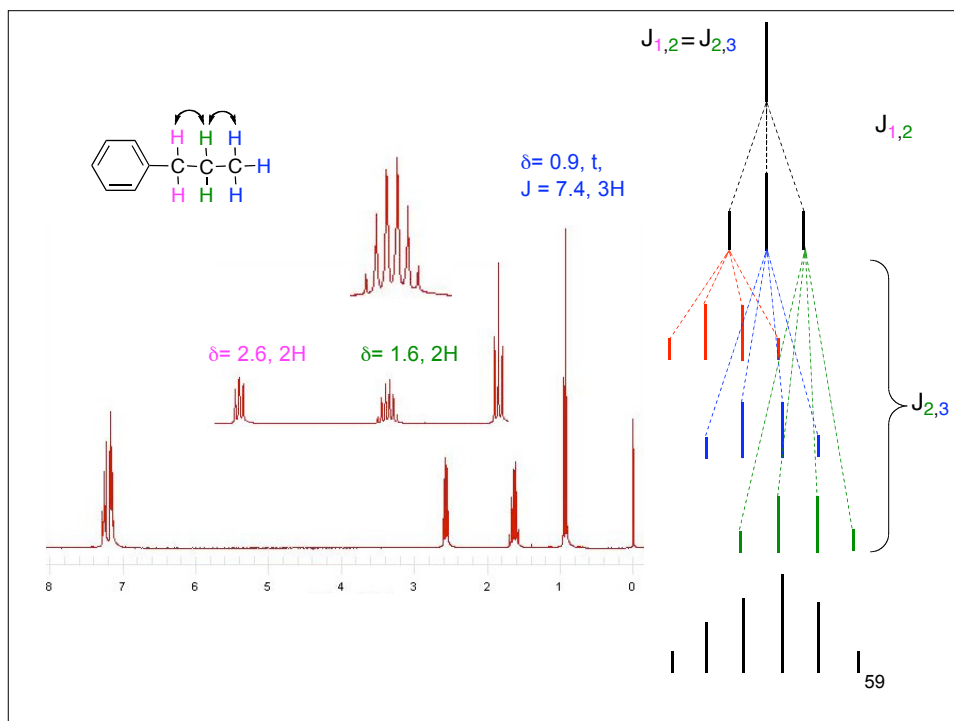
13.10: Splitting Patterns: Pairs of Doublets



57

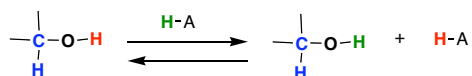
13.11: Complex Splitting Patterns: when a protons is adjacent to more than one set of non-equivalent protons, they will split independently





13.12: ¹H NMR Spectra of Alcohols

Usually no spin-spin coupling between the O–H proton and neighboring protons on carbon due to exchange reaction



The chemical shift of the -OH proton occurs over a large range (2.0 - 5.5 ppm). This proton usually appears as a broad singlet. It is not uncommon for this proton not to be observed.

13.13: NMR and Conformation (please read)

NMR is like a camera with a slow shutter speed. What is observed is a weighted time average of all conformations present.

60

Summary of ^1H - ^1H spin-spin coupling

- chemically equivalent protons do not exhibit spin-spin coupling to each other.
- the resonance of a proton that has n equivalent protons on the adjacent carbon is split into $n+1$ peaks (multiplicity) with a coupling constant J .
- protons that are coupled to each other have the same coupling constant
- non-equivalent protons will split a common proton independently: complex coupling.

Spin-spin coupling is normally observed between nuclei that are one, two and three bonds away. Four-bond coupling can be observed in certain situations (i.e., aromatic rings), but is not common.

61

Summary of ^1H -NMR Spectroscopy

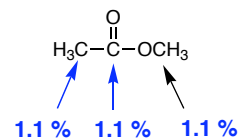
- the number of proton resonances equals the number of non-equivalent protons
- the chemical shift (δ , ppm) of a proton is diagnostic of the chemical environment (shielding and deshielding)
- Integration: number of equivalent protons giving rise to a resonance
- spin-spin coupling is dependent upon the number of equivalent protons on the adjacent carbon(s)

62

¹³C NMR Spectroscopy:

Natural Abundance

¹H 99.9% (I= 1/2) ¹²C 98.9% (I= 0)
¹³C 1.1% (I= 1/2)



$$\Delta E = \frac{\gamma B_o h}{2 \pi}$$

B_o = external magnetic field strength

γ = magnetogyric ratio

¹H= 26,752

¹³C= 6.7

¹³C is a much less sensitive nuclei than ¹H for NMR spectroscopy

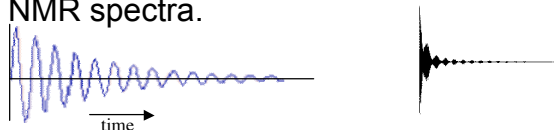
New techniques (hardware and software) has made ¹³C NMR routine

- Pulsed NMR techniques (FT or time domain NMR)
- Signal averaging (improved signal to noise)

Animation: http://mutuslab.cs.uwindsor.ca/schurko/nmrcourse/animations/eth_anim/puls_evol.gif

63

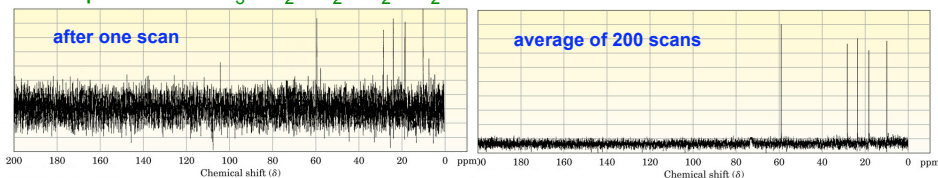
Fourier Transform (FT) deconvolutes all of the FID's and gives an NMR spectra.



Signal-averaging: pulsed NMR allows for many FID's (NMR spectra) to be accumulated over time. These FID's are added together and averaged. Signals (resonances) build up while the "noise" is random and cancels out during the averaging.

Enhanced signal to noise ratio and allows for NMR spectra to be collected on insensitive nuclei such as ¹³C and small samples.

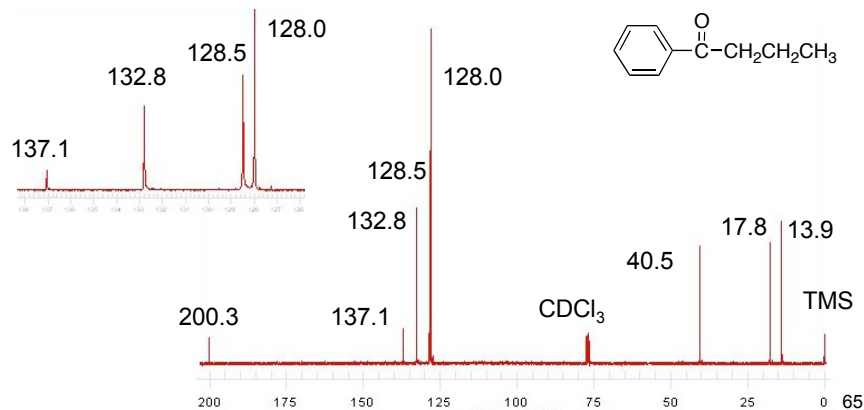
¹³C-spectra of CH3CH2CH2CH2CH2OH



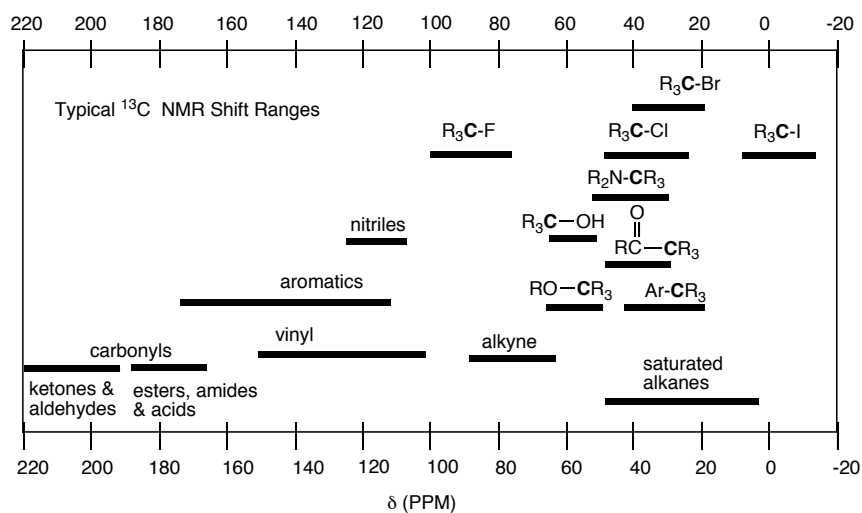
64

Chemical shifts give an idea of the chemical and electronic environment of the ^{13}C nuclei due to shielding and deshielding effects range: 0 - 220 ppm from TMS

^{13}C NMR spectra will give a map of the carbon framework. The number of resonances equals the number of non-equivalent carbons.



Chemical Shift Range of ^{13}C



Note the carbonyl range

66

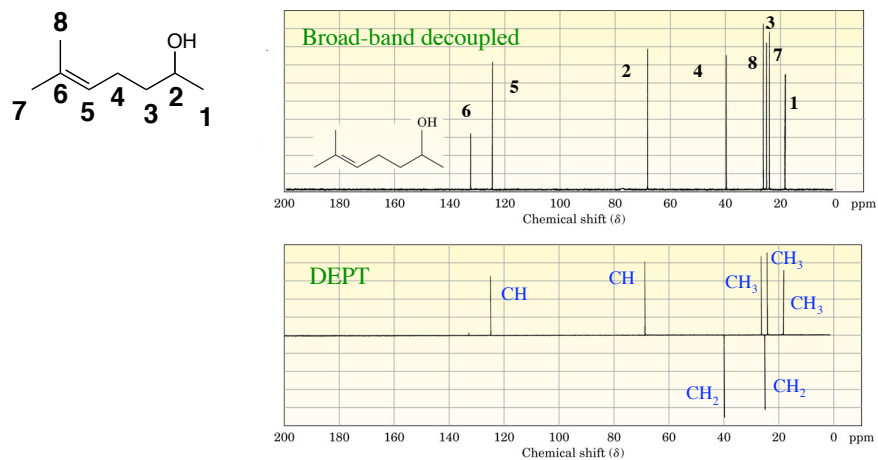
13.18: Using DEPT to Count Hydrogens Attached to ^{13}C

^1H - ^{13}C spin-spin coupling: spin-spin coupling tells how many protons are attached to the ^{13}C nuclei. (i.e., primary, secondary tertiary, or quaternary carbon)

^{13}C spectra are usually collected with the ^1H - ^{13}C coupling "turned off" (broad band decoupled). In this mode all ^{13}C resonances appear as singlets.

DEPT spectra (Distortionless Enhancement by Polarization Transfer) a modern ^{13}C NMR spectra that allows you to determine the number of attached hydrogens.

67



CH_2 's give negative resonances

CH 's and CH_3 's give positive resonances

Quaternary carbon (no attached H's) are not observed

13.19: 2D NMR: COSY and HETCOR (please read)

68

Solving Combined Spectra Problems:

Mass Spectra:

Molecular Formula

Nitrogen Rule → # of nitrogen atoms in the molecule

~~M+1 peak → # of carbons~~

Degrees of Unsaturation: # of rings and/or π -bonds

Infrared Spectra:

Functional Groups

C=O

O-H

C=C

N-H

C≡C

CO-OH

C≡N

^1H NMR:

Chemical Shift (δ) → chemical environment of the H's

Integration → # of H's giving rise to the resonance

Spin-Spin Coupling (multiplicity) → # of non-equivalent H's on the adjacent carbons (vicinal coupling).

^{13}C NMR:

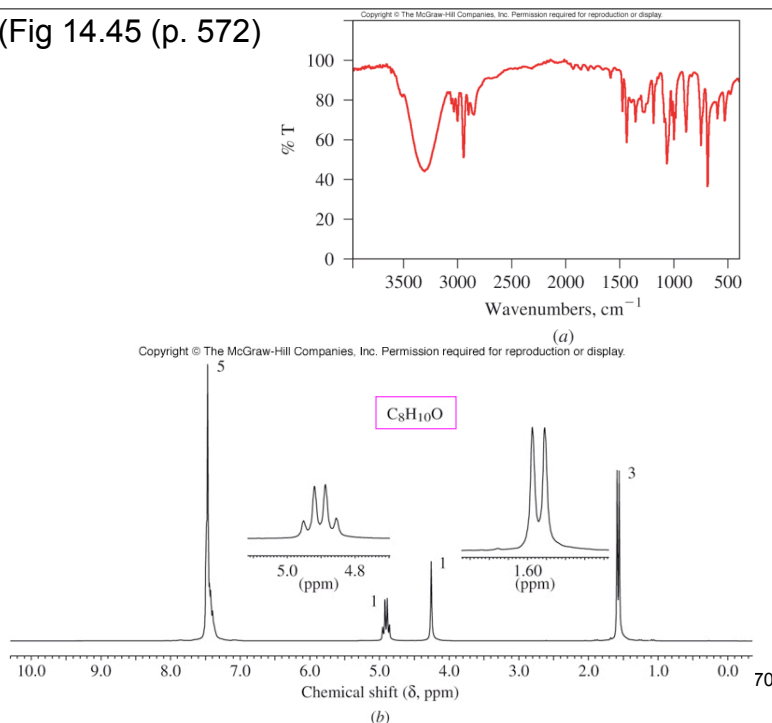
of resonances → symmetry of carbon framework

Type of Carbonyl

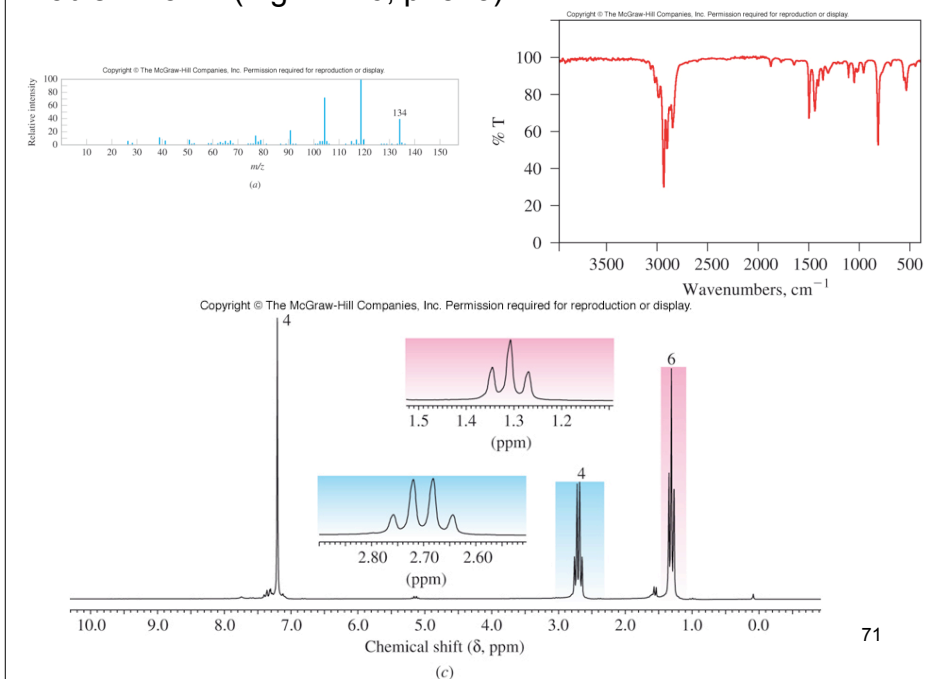
Each piece of evidence gives a fragment (puzzle piece) of the structure. Piece the puzzle together to give a proposed structure. The proposed structure should be consistent with all the evidence.

69

13.41 (Fig 14.45 (p. 572))



Problem 13.42 (Fig. 14.46, p. 573)



13.43 (Fig. 13.47, p. 574): $C_5H_{10}O$

