



Organic Chemistry

Tenth Edition

T. W. Graham Solomons
Craig B. Fryhle

Welcome to CHM 2211
Organic Chemistry II
Chapters 2 (IR), 9, 13-20.

Chapter 2 and Chapter 9

Spectroscopy

(interaction of molecule with electromagnetic radiations)

Chapter 2: Infrared Spectroscopy (IR)

Chapter 9: Nuclear Magnetic Resonance (NMR)

Chapter 9: Mass Spectrometry (MS)

Chapter 13: Ultraviolet- visible Spectroscopy (UV-VIS)

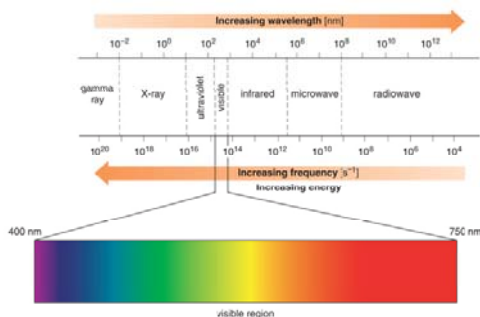
Ch. 2 - 2

Spectroscopy

Electromagnetic Radiation

- The different forms of electromagnetic radiation make up the electromagnetic spectrum.

Figure 14.7 The electromagnetic spectrum



* Visible light occupies only a small region of the electromagnetic spectrum.

Infrared Spectroscopy

Electromagnetic Radiation

- The electromagnetic spectrum is arbitrarily divided into different regions.

- Wavelength (λ) and frequency (ν) are inversely related:

Wavelength increases as frequency decreases.

Frequency increases as wavelength decreases.

$$\nu = c/\lambda$$

[C= speed of light]

- The energy (E) of a photon is directly proportional to its frequency and therefore reversely proportional to wavelength:

$$E = h\nu$$

[h = Planck's constant]

Infrared Spectroscopy

Background

- Infrared (IR) spectroscopy is used to identify the functional groups in a compound. It uses IR radiation as the energy source.
- Frequencies in IR spectroscopy are reported using a unit called wavenumber ($\tilde{\nu}$):

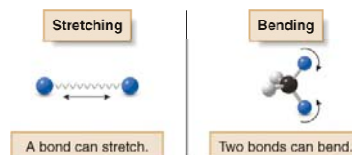
$$\tilde{\nu} = 1/\lambda$$

- Wavenumber is inversely proportional to wavelength and is given in reciprocal centimeters (cm^{-1}).
- Therefore, frequency (and energy) increases as the wavenumber increases.

Using the wavenumber scale, IR absorptions for all organic compounds (functional groups) occur from 4000 cm^{-1} to 400 cm^{-1} .

Infrared Spectroscopy

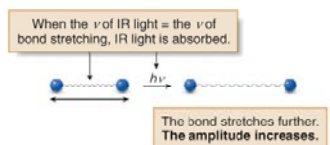
- Absorption of IR light causes changes in the vibrational motions of a molecule.
- The different vibrational modes available to a molecule include stretching and bending modes.



- The vibrational modes of a molecule occur only at specific frequencies which correspond to the frequency of IR light.

Infrared Spectroscopy

- When the frequency of IR light matches the frequency of a particular vibrational mode, the IR light is absorbed, causing the amplitude of the particular bond stretch or bond bend to increase.

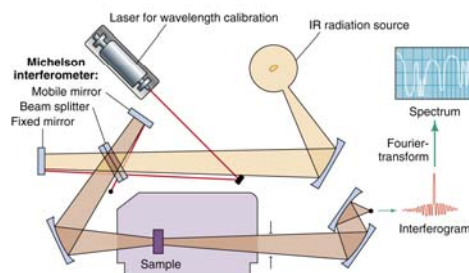


- Different kinds of bonds vibrate at different frequencies, so they absorb different frequencies of IR light.
- IR spectroscopy distinguishes between the different kinds of bonds in a molecule, so it is possible to determine the functional groups present.

Infrared Spectroscopy

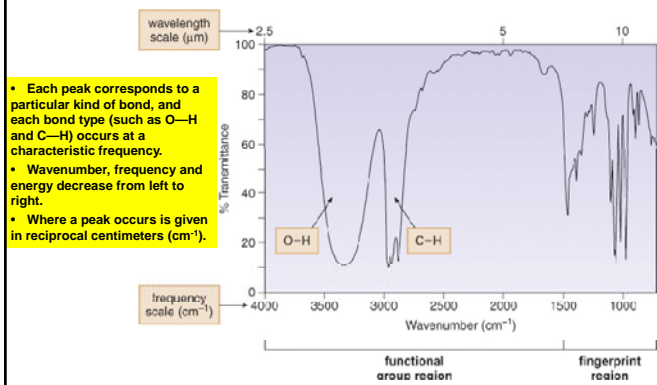
Characteristics of an IR Spectrum

- In an IR spectrometer, light passes through a sample.
- Frequencies that match the vibrational frequencies are absorbed, and the remaining light is transmitted to a detector.
- An IR spectrum is a plot of the amount of transmitted light versus its wavenumber.



Infrared Spectroscopy

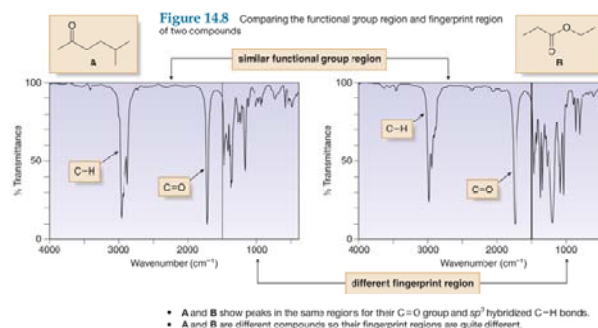
- Let us now consider the IR spectrum of 1-propanol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$.
- Always look for the characteristic peak of the functional group present in the molecule
- Characteristics of an IR Spectrum for 1-Propanol are the specific absorption of the OH group:



Infrared Spectroscopy

Characteristics of an Infrared Spectrum

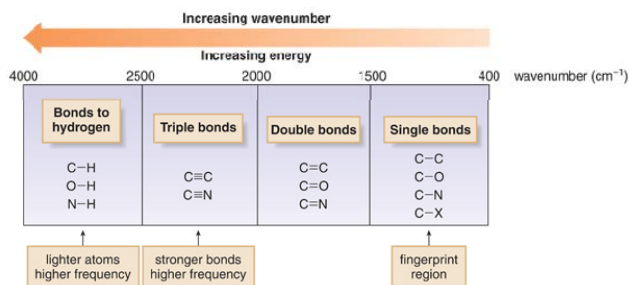
- The IR spectrum is divided into two regions: the functional group region (at $\geq 1500 \text{ cm}^{-1}$), and the fingerprint region (at $< 1500 \text{ cm}^{-1}$)
- Please note a characteristic peak for a carbonyl from from ketone and ester at $\sim 1700 \text{ cm}^{-1}$.



Infrared Spectroscopy

- Bonds absorb in four predictable regions of an IR spectrum.

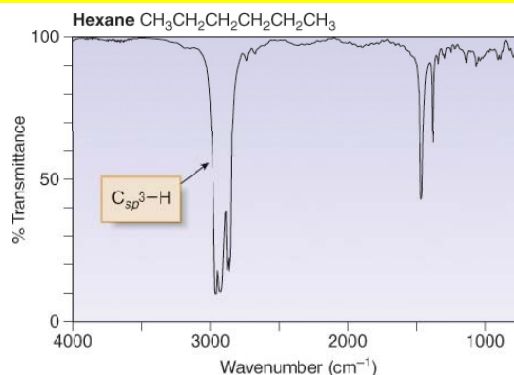
Summary of the four regions of the IR spectrum



Infrared Spectroscopy

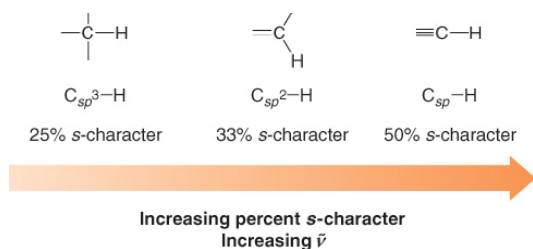
IR Absorptions in Hydrocarbons - Alkane

- Hexane has only C—C single bonds and sp^3 hybridized C atoms. Therefore it has only one major absorption at $3000\text{--}2850 \text{ cm}^{-1}$.



Infrared Spectroscopy

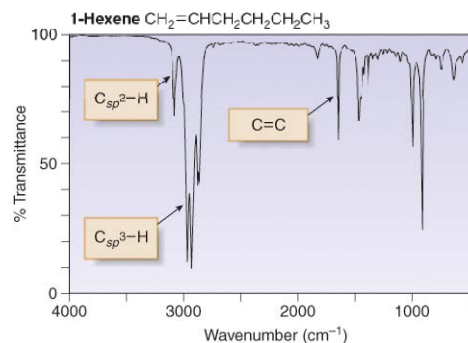
- Even subtle differences that affect bond strength affect the frequency of an IR absorption.



Infrared Spectroscopy

IR Absorptions in Hydrocarbons - Alkene

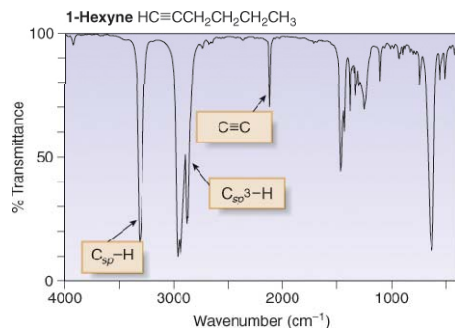
1-Hexene has a C=C and $C_{sp^2}-H$, in addition to sp^3 hybridized C atoms. Therefore, there are three major absorptions: $C_{sp^2}-H$ at 3150-3000 cm^{-1} ; $C_{sp^3}-H$ at 3000-2850 cm^{-1} ; C=C at 1650 cm^{-1} .



Infrared Spectroscopy

IR Absorptions in Hydrocarbons - Alkynes

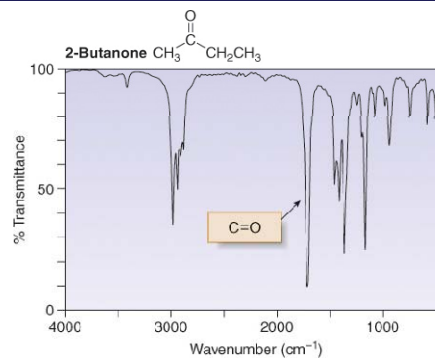
1-Hexyne has a C≡C and $C_{sp}-H$, in addition to sp^3 hybridized C atoms. Therefore, there are three major absorptions: $C_{sp}-H$ at 3300 cm^{-1} ; $C_{sp^3}-H$ at 3000-2850 cm^{-1} ; C≡C at 2250 cm^{-1} .



Infrared Spectroscopy

IR Absorptions in Oxygen Containing Compounds

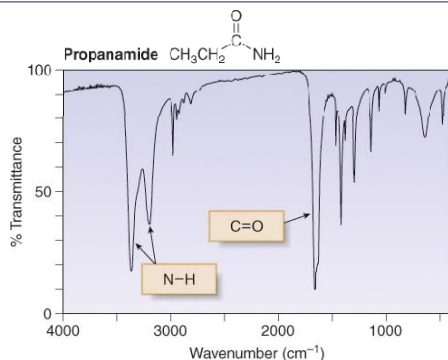
The C=O groups in the ketones as well as aldehydes and esters show a strong absorption at ~1700 cm^{-1} .



Infrared Spectroscopy

IR Absorptions in Nitrogen Containing Compounds - Amides

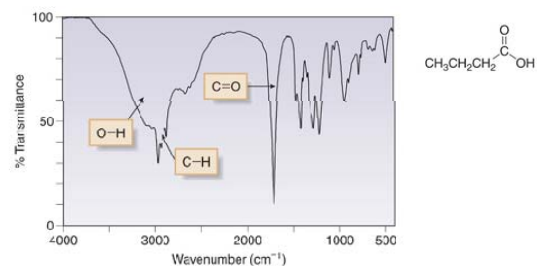
The amide exhibits absorptions above 1500 cm^{-1} for both its N—H and C=O groups: N—H (two peaks) at 3200 and 3400 cm^{-1} ; C=O at 1660 cm^{-1} .



Infrared Spectroscopy

Carboxylic Acids and the Acidity of the O—H Bond

Figure 19.4 The IR spectrum of butanoic acid, $\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$



- A strong C=O absorption occurs at 1712 cm^{-1} .
- The broad O—H absorption ($2500\text{--}3500\text{ cm}^{-1}$) nearly obscures the C—H peak at $\sim 3000\text{ cm}^{-1}$.

Nuclear Magnetic Resonance (NMR) Spectroscopy

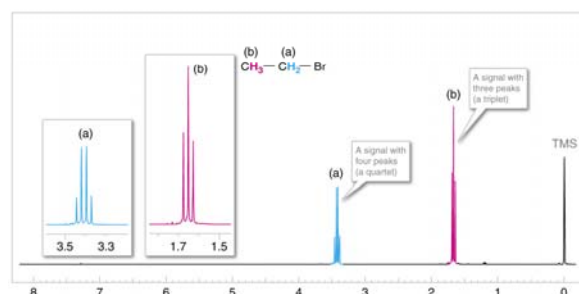
- Two common types of NMR spectroscopy are used to characterize organic structure:
 - ^1H NMR is used to determine the type and number of H atoms in a molecule;
 - ^{13}C NMR is used to determine the type of carbon atoms in the molecule.
- The source of energy in NMR is radio waves which have long wavelengths, and thus low energy and frequency.
- When this low-energy radio waves interact with a molecule, they can change the nuclear spins of some elements, including ^1H and ^{13}C .

Nuclear Magnetic Resonance Spectroscopy

^1H NMR is used to determine the type and number of H atoms in a molecule

A typical ^1H NMR spectra of 1-bromopropane is shown here: It has four features:

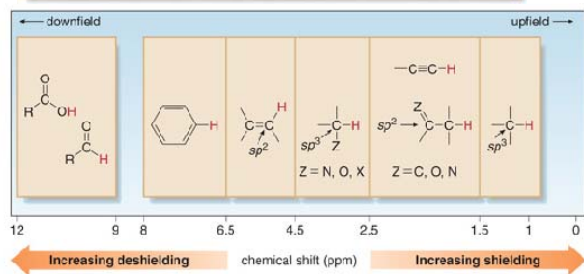
- (1) The number of signals in the spectrum tell us how many different set of protons are in the molecule,
- (2) The position of the signal in the spectrum along x-axis tell us about magnetic environment,
- (3) The area under the signal tell us how many protons there are in each set being measured,
- (4) The multiplicity (or splitting pattern) of each signal tell us about the number of protons on atoms adjacent to the one whose signal is being measured.



NMR Spectroscopy - Chemical Shift Values

- The position of a signal on the x axis of NMR spectrum is called **chemical shift**.
- It is measured in ppm, according to the following equation:

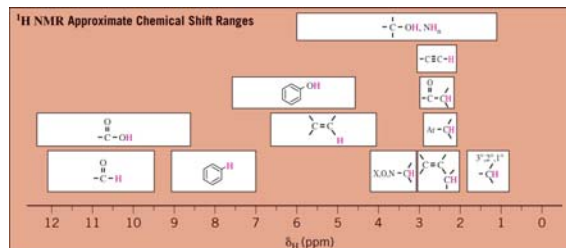
$$\text{chemical shift (in ppm on the } \delta \text{ scale)} = \frac{\text{observed chemical shift (in Hz) downfield from TMS}}{\nu \text{ of the NMR spectrometer (in MHz)}}$$



- Shielded protons absorb at lower chemical shift (to the right).
- Deshielded protons absorb at higher chemical shift (to the left).

NMR Spectroscopy - Chemical Shift Values

- Protons in a given environment absorb in a predictable region in an NMR spectrum.

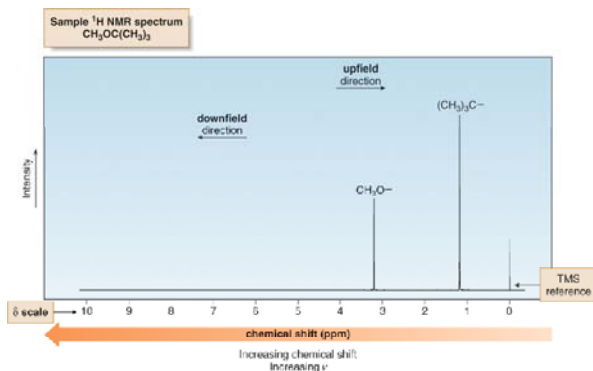


- Most protons absorb between 0-10 ppm.
- The terms "upfield" and "downfield" describe the relative location of peaks. Upfield means to the right. Downfield means to the left.
- NMR absorptions are measured relative to the position of a reference peak at 0 ppm on the δ scale due to tetramethylsilane (TMS). TMS is a volatile inert compound that gives a single peak upfield from typical NMR absorptions.

Nuclear Magnetic Resonance Spectroscopy

^1H NMR—The Spectrum

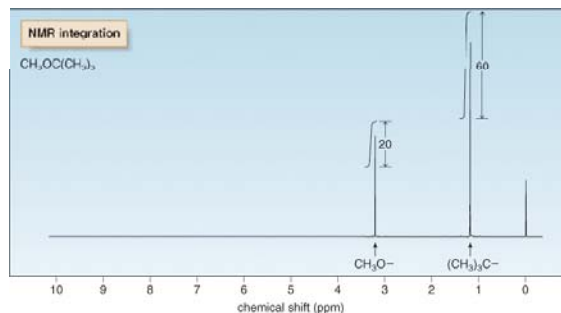
- An NMR spectrum is a plot of the intensity of a peak against its chemical shift, measured in parts per million (ppm).



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Intensity of Signals (Integration)

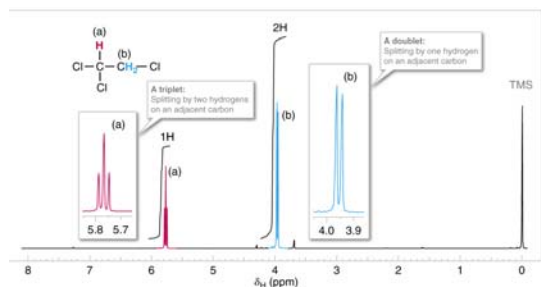
- The area under an NMR signal is proportional to the number of absorbing protons.
- An NMR spectrometer automatically **integrates** the area under the peaks, and prints out a stepped curve (the integral) on the spectrum.
- The height of each step is proportional to the area under the peak, which in turn is proportional to the number of absorbing protons.



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Spin-Spin Splitting

The signal from a given proton will be split by the effect of magnetic fields associated with protons on neighboring carbons.



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Spin-Spin Splitting

General rule which describes the splitting patterns commonly seen in the ^1H NMR spectra of organic compounds is as follow:

A number of peaks from vicinal coupling in set is equalled

$$n + 1$$

Where n is the number of vicinal hydrogens [at nearby (adjacent) carbons] that are nonequivalent to those producing the signal



H_a and H_b are on adjacent carbons.

Please note that H_a and H_b are separated by **three σ bonds**. They are called **vicinal protons** because they are on adjacent carbons. Three bond coupling between them is called **vicinal coupling**.

Splitting is **not generally observed** between protons separated by **more than three σ bonds**.

NMR Spectroscopy - ^1H NMR—Spin-Spin Splitting

Whenever two (or three) different sets of adjacent protons are equivalent to each other, use the $n + 1$ rule to determine the splitting pattern.

In general we have to ask only one question and then use $N + 1$ rule.

Question. How many protons are there on the adjacent carbon or carbons?

Answer is $N = 6$: Therefore, we should expect 7 lines in the multiplet for H at CHBr carbon

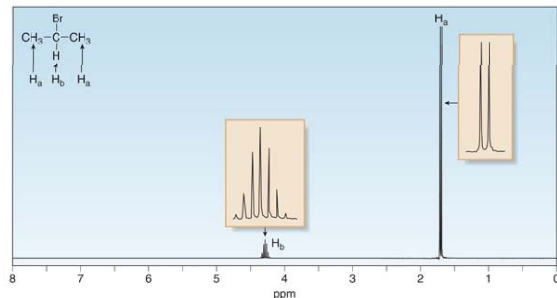
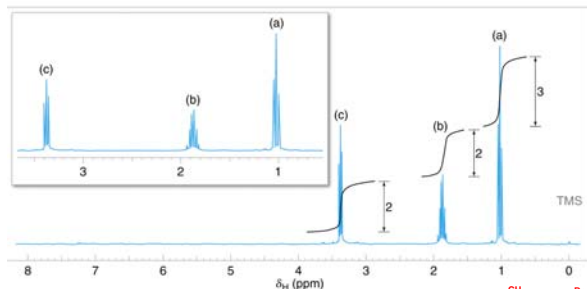


TABLE 15.4 Common Splitting Patterns Observed in ^1H NMR

Example	Pattern	Analysis (H_a and H_b are not equivalent.)
[1]		<ul style="list-style-type: none"> H_a: one adjacent H_b proton \rightarrow two peaks \rightarrow a doublet H_b: one adjacent H_a proton \rightarrow two peaks \rightarrow a doublet
[2]		<ul style="list-style-type: none"> H_b: two adjacent H_a protons \rightarrow three peaks \rightarrow a triplet H_a: one adjacent H_b proton \rightarrow two peaks \rightarrow a doublet
[3]		<ul style="list-style-type: none"> H_b: two adjacent H_a protons \rightarrow three peaks \rightarrow a triplet H_a: two adjacent H_b protons \rightarrow three peaks \rightarrow a triplet
[4]		<ul style="list-style-type: none"> H_b: three adjacent H_a protons \rightarrow four peaks \rightarrow a quartet; the relative area under the peaks of a quartet is 1:3:3:1. H_a: two adjacent H_b protons \rightarrow three peaks \rightarrow a triplet
[5]		<ul style="list-style-type: none"> H_b: three adjacent H_a protons \rightarrow four peaks \rightarrow a quartet H_a: one adjacent H_b proton \rightarrow two peaks \rightarrow a doublet

NMR Spectroscopy – Interpretation of Proton NMR Spectra: Chapter 9.3

Consider the spectrum of alkyl bromides with molecular formula C_3H_7Br .

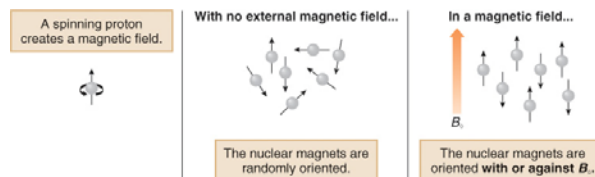


1. Count the number of signal!
2. Correlate chemical shift with possible structural environments!
3. Determine the relative area of each signal!
4. Interpret the splitting pattern!
5. Join the fragments to make a molecule which structure would be consistent with data!

Nuclear Magnetic Resonance Spectroscopy

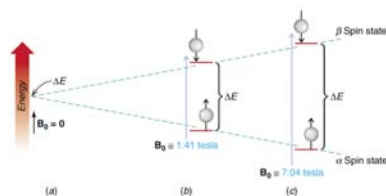
Nuclear Spin – The Origin of the Signal

- When a charged particle such as a proton spins on its axis, it creates a magnetic field. **Thus, the nucleus can be considered to be a tiny bar magnet.**
- Normally, these tiny bar magnets are randomly oriented in space. However, in the presence of a magnetic field B_0 , they are oriented with or against this applied field.
- The energy difference between these two states is very small (<0.1 cal).



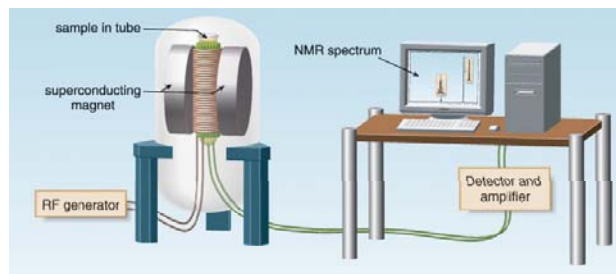
Nuclear Magnetic Resonance Spectroscopy

- In a magnetic field, there are now two energy states for a proton: **a lower energy state with the nucleus aligned in the same direction as B_0** ; and a higher energy state with the nucleus aligned opposed to B_0 .
- When an external energy source ($h\nu$) that matches the energy difference (ΔE) between these two states is applied, energy is absorbed, causing the nucleus to “spin flip” from one orientation to another.
- The energy difference between these two nuclear spin states corresponds to the low frequency RF region of the electromagnetic spectrum.



Nuclear Magnetic Resonance Spectroscopy

Schematic of an NMR spectrometer

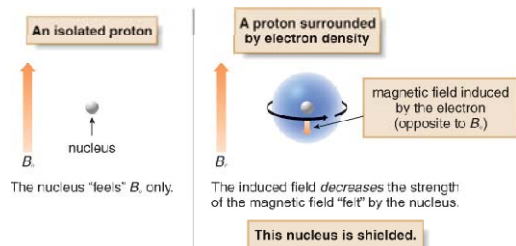


- Protons (which are the nuclei of hydrogen atoms) that are in different environments absorb at slightly different frequencies, so they are distinguishable by NMR.
- The frequency at which a particular proton absorbs is determined by the strength of the magnetic field generated by the electrons around it.
- NMR spectrometers are referred to as 300 MHz or 500 MHz instruments, and so forth, depending on the frequency of the RF radiation used for resonance.
- These spectrometers use powerful magnets to create a small but measurable energy difference between two possible spin states.

Nuclear Magnetic Resonance Spectroscopy

Shielding and Deshielding of Protons

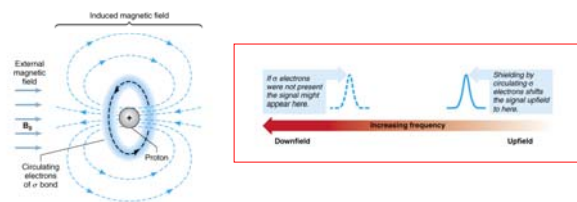
- In the vicinity of the nucleus, the magnetic field generated by the circulating electron **decreases the external magnetic field that the proton "feels"**.
- Since the electron experiences a lower magnetic field strength, it needs a lower frequency to achieve resonance. Lower frequency is to the right in an NMR spectrum, toward a lower chemical shift, so **shielding** shifts the absorption upfield.



Nuclear Magnetic Resonance Spectroscopy

Shielding and Deshielding of Protons

- The small magnetic field generated by electrons is called an **induced field**. Since the actual magnetic field sensed by proton is slightly less than the external field, the electrons are said to **shield the protons** and the signal is **shifted upfield** since lower energy is needed to achieve resonance.

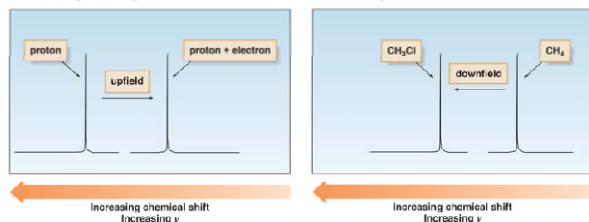


Nuclear Magnetic Resonance Spectroscopy

Position of Signals - Shielding and Deshielding of Protons Relation to Chemical Shift

Figure 15.3 How chemical shift is affected by electron density around a nucleus

- [a] Shielding effects**
- An electron shields the nucleus.
 - The absorption shifts upfield.
- [b] Deshielding effects**
- Decreased electron density deshields a nucleus.
 - The absorption shifts downfield.



Nuclear Magnetic Resonance Spectroscopy

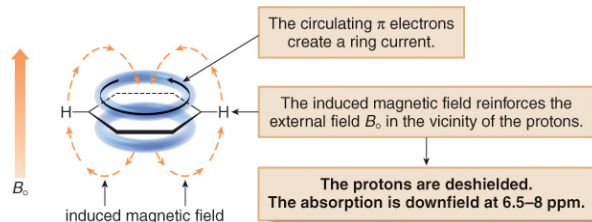
Position of Signals - Shielding and Deshielding of Protons Relation to Chemical Shift

- A shielded nucleus**
- The nucleus "feels" a smaller resultant field.
 - a larger induced magnetic field
 - As the electron density around the nucleus increases, the nucleus feels a smaller resultant magnetic field, so a lower frequency is needed to achieve resonance.
 - The absorption shifts upfield.
- A deshielded nucleus**
- The nucleus "feels" a larger resultant field.
 - a smaller induced magnetic field
 - As the electron density around the nucleus decreases, the nucleus feels a larger resultant magnetic field, so a higher frequency is needed to achieve resonance.
 - The absorption shifts downfield.

Nuclear Magnetic Resonance Spectroscopy

Position of Signals - Shielding and Deshielding of Protons Aromatic Compounds

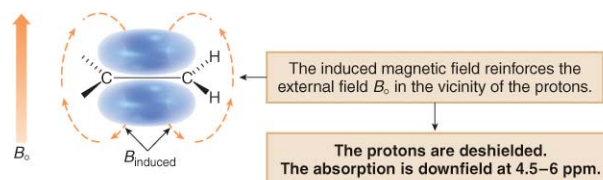
- In a magnetic field, the six π electrons in benzene circulate around the ring creating a **ring current**.
- The magnetic field induced by these moving electrons **reinforces** the applied magnetic field in the vicinity of the protons.
- The protons thus **feel a stronger magnetic field** and a **higher frequency is needed for resonance**. Thus they are **deshielded** and absorb **downfield**.



Nuclear Magnetic Resonance Spectroscopy

Position of Signals - Shielding and Deshielding of Protons Alkenes

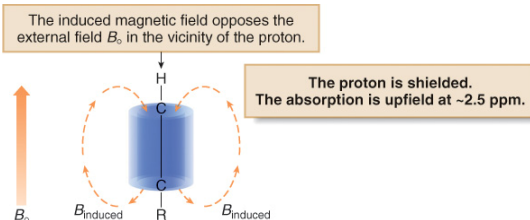
- In a magnetic field, the loosely held π electrons create a magnetic field that reinforces the applied field in the vicinity of the protons.
- Since the protons now feel a stronger magnetic field, they require a higher frequency for resonance. Thus the protons are deshielded and the absorption is downfield.



Nuclear Magnetic Resonance Spectroscopy

Position of Signals - Shielding and Deshielding of Protons Alkynes

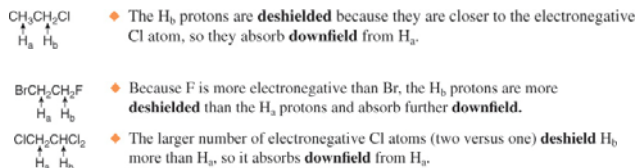
- In a magnetic field, the π electrons of a carbon-carbon triple bond are induced to circulate, but in this case the induced magnetic field opposes the applied magnetic field (B_0).
- Thus, the proton feels a weaker magnetic field, so a lower frequency is needed for resonance. The nucleus is shielded and the absorption is upfield.



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Position of Signals – Effect of electronegativity

- Protons near electronegative atoms are deshielded, so they absorb downfield
- This **deshielded** nucleus experiences a higher magnetic field strength, so it needs a higher frequency to achieve resonance.
- Higher frequency is to the left in an NMR spectrum, toward higher chemical shift—so deshielding shifts an absorption downfield..



Nuclear Magnetic Resonance Spectroscopy

Summary —Shielding and Chemical Shift Values

TABLE 15.2 Effect of π Electrons on Chemical Shift Values

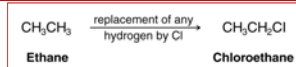
Proton type	Effect	Chemical shift (ppm)
	highly deshielded	6.5–8
	deshielded	4.5–6
$\text{—C}\equiv\text{C—H}$	shielded	~2.5

Aldehyde protons are highly deshielded and resonates at around 9.8 ppm. Why?

Nuclear Magnetic Resonance Spectroscopy

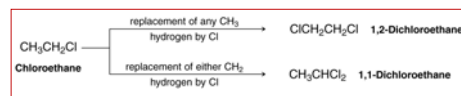
Chemical Shift Equivalent and Nonequivalent Protons. Homotopic and Heterotopic Hydrogens

- How do we decide whether two or more protons in a molecule are in identical environment (chemical, magnetic)?- **Atom replacement method**



Replacing any one of the six hydrogens of ethane by different atoms gives the **same** compound. All six hydrogens are **homotopic** and therefore chemical shift equivalent.

Homotopic hydrogen have identical environment and will have the same chemical shift. They are said to be chemical shift equivalent.



Thus, replacing of hydrogens from methyl OR methylene group yields **TWO different** compounds. Chloroethane has two sets of hydrogens that are **heterotopic** to each others

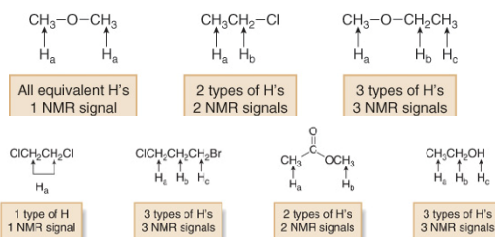
Heterotopic atoms have different chemical shift and are not chemical shift equivalent

Nuclear Magnetic Resonance Spectroscopy

Chemical Shift Equivalent and Nonequivalent Protons. Homotopic and Heterotopic Hydrogens

Number of Signals

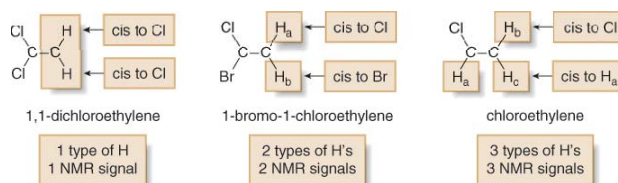
- The number of NMR signals equals the number of different types of protons in a compound.
- Protons in different environments give different NMR signals.
- Equivalent protons (**chemically and magnetically**) give the same NMR signal.



Nuclear Magnetic Resonance Spectroscopy

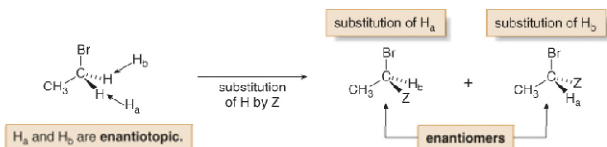
^1H NMR—Number of Signals

- However, two H atoms on a ring or double bond protons are equivalent only if they are **cis (or trans)** to the same groups.



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Enantiotopic and Diastereotopic Protons.

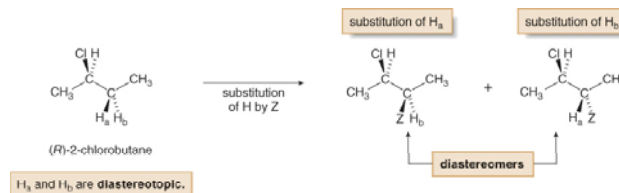


- When substitution of two H atoms by Z forms enantiomers, the two H atoms are equivalent and give a single NMR signal. These two H atoms are called *enantiotopic* protons.

Enantiotopic hydrogens have the same chemical shift and appear in the same signal.

Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Enantiotopic and Diastereotopic Protons.



- When substitution of two H atoms by Z forms diastereomers, the two H atoms are not equivalent, and give two NMR signals. These two H atoms are called *diastereotopic* protons.

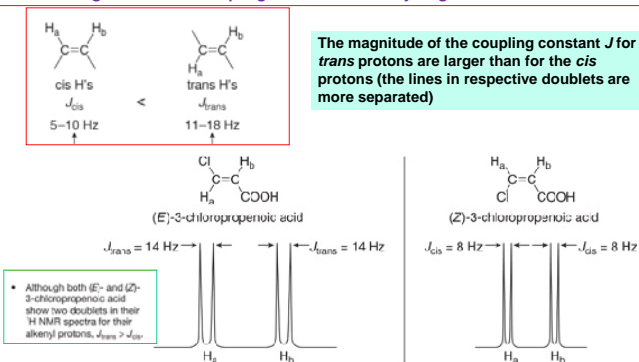
Diastereotopic hydrogens have different chemical shifts and will give different signals.

Nuclear Magnetic Resonance Spectroscopy

^1H NMR Spectra for alkenes:

How can we distinguish between E and Z isomers?

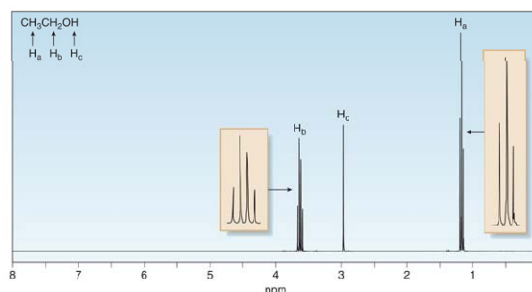
Different magnitude of the coupling constant for the hydrogen in *trans* and *cis* relation



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—OH Protons: The Spectra of alcohols.

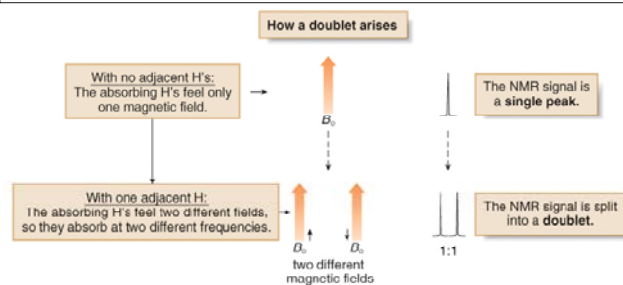
- Under usual conditions, an OH proton does not split the NMR signal of adjacent protons.
- The signal due to an OH proton is not split by adjacent protons.



Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Spin-Spin Splitting: Doublet formation

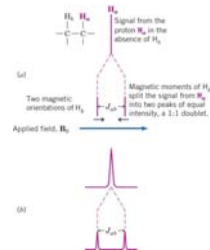
The frequency difference, measured in Hz between two peaks of the doublet is called the **coupling constant, J** .



♦ One adjacent proton splits an NMR signal into a doublet.

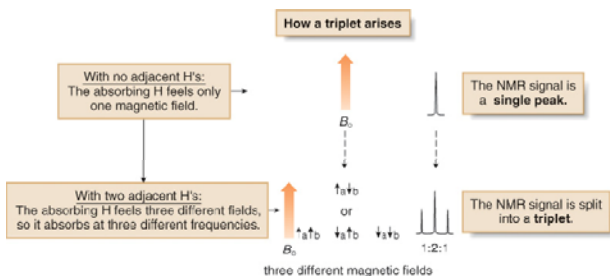
→ The magnetic field sensed by a proton (H_a) being observed is affected by the magnetic moment of an adjacent proton (H_b)

- ▮ A proton (H_b) can be aligned with the magnetic field or against the magnetic field, resulting in two energy states for H_b .
- ▮ The observed proton (H_a) senses the two different magnetic moments of H_b as a slight change in the magnetic field; one magnetic moment reinforces the external field and one subtracts from it.
- ▮ The signal for H_a is split into a doublet with a 1:1 ratio of peak areas.
- ▮ The magnitude of the splitting is called the coupling constant J_{ab} and is measured in Hertz (Hz).



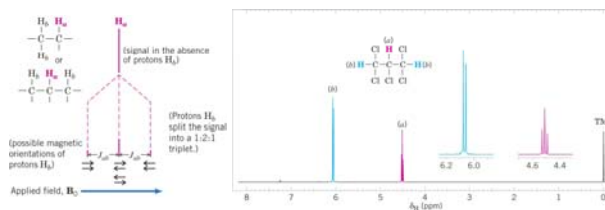
Nuclear Magnetic Resonance Spectroscopy

^1H NMR—Spin-Spin Splitting: Triplet formation



→ When two adjacent protons H_b are coupled to H_a , there are four possible combinations of the magnetic moments for the two H_b s

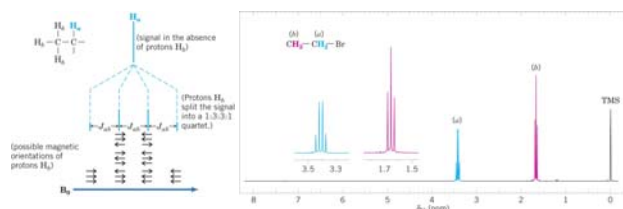
- ▮ Two of these combinations involve pairings of magnetic moments that cancel each other, causing no net displacement of signal.
- ▮ One combination of magnetic moments reinforces and another subtracts from the applied magnetic field.
- ▮ H_a is split into a triplet having a 1:2:1 ratio of signal areas.



¹H NMR—Spin-Spin Splitting: Quartet formation

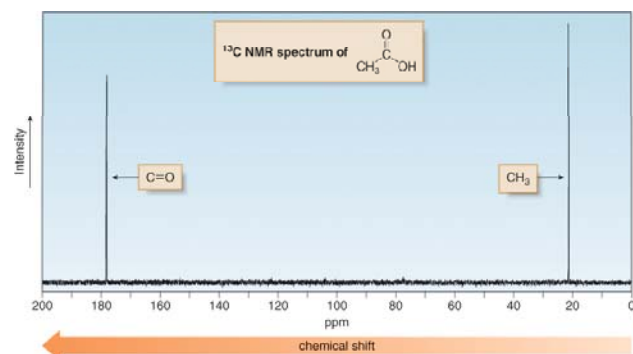
→ When three adjacent protons are coupled to H_a, there are 10 possible combinations of the magnetic moments for the H_bs

Four unique orientations exist and so H_a is split into a quartet with intensities 1:4:6:4:1

**Nuclear Magnetic Resonance Spectroscopy - ¹³C NMR**

¹³C signals are not split. Each type of carbon atom appears as a single peak

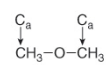
One peak for each magnetically distinct carbon

**NMR Spectroscopy- ¹³C NMR**

- The two features of a ¹³C NMR spectrum that provide the most structural information are the **number of signals** observed and the **chemical shifts** of those signals.
- The lack of splitting in a ¹³C spectrum is a consequence of the low natural abundance of ¹³C.
- Recall that splitting occurs when two NMR active nuclei—like two protons—are close to each other. Because of the low natural abundance of ¹³C nuclei (1.1%), the chance of two ¹³C nuclei being bonded to each other is very small (0.01%), and so no carbon-carbon splitting is observed.
- A ¹³C NMR signal can also be split by nearby protons. This ¹H-¹³C splitting is usually eliminated from the spectrum by using an instrumental technique that decouples the proton-carbon interactions, so that every peak in a ¹³C NMR spectrum appears as a singlet.

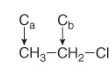
¹³C NMR Spectroscopy —Number of Signals

- The number of signals in a ¹³C spectrum gives the number of different types of carbon atoms in a molecule.
- Because ¹³C NMR signals are not split, the number of signals/lines in the ¹³C spectrum equals number of nonequivalent carbons.
- In contrast to the ¹H NMR situation, peak intensity is not proportional to the number of absorbing carbons, so **¹³C NMR signals are not integrated.**

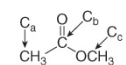


1 ¹³C NMR signal

Both C's are equivalent.



2 ¹³C NMR signals

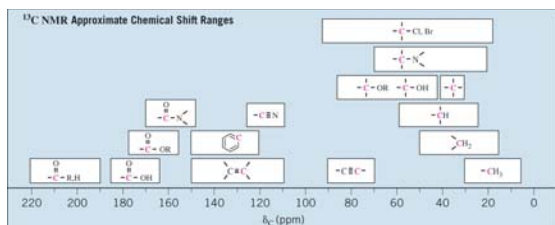


3 ¹³C NMR signals

¹³C Chemical Shifts

→ Just as in ¹H NMR spectroscopy, chemical shifts in ¹³C NMR depend on the electron density around the carbon nucleus

- Decreased electron density causes the signal to move downfield (*deshielding*)
- Increased electron density causes the signal to move upfield (*shielding*)



→ Because of the wide range of chemical shifts, it is rare to have two ¹³C peaks coincidentally overlap

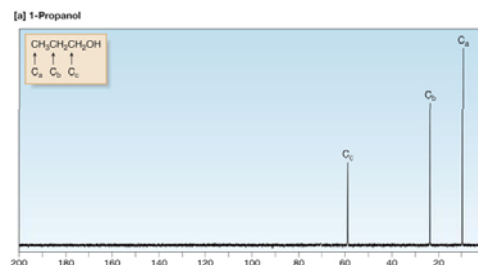
→ A group of 3 peaks at δ 77 comes from the common NMR solvent deuteriochloroform and can be ignored

Nuclear Magnetic Resonance Spectroscopy

¹³C NMR—Number of Signals

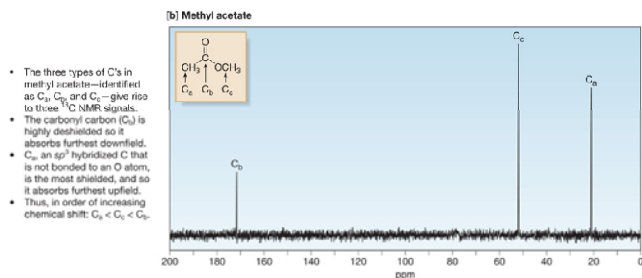
Figure 15.14
Representative ¹³C NMR spectra

- The three types of C's in 1-propanol—identified as C_α, C_β, and C_γ—give rise to three ¹³C NMR signals.
- Deshielding increases with increasing proximity to the electronegative O atom, and the absorption shifts downfield, thus, in order of increasing chemical shift: C_γ < C_β < C_α.



Nuclear Magnetic Resonance Spectroscopy

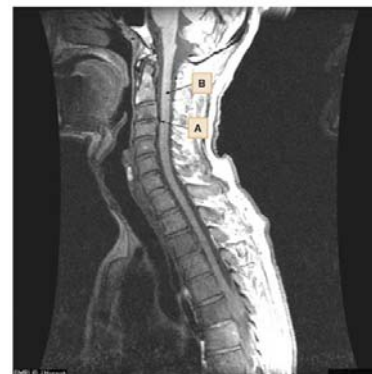
¹³C NMR—Number of Signals



Nuclear Magnetic Resonance Spectroscopy

Figure 15.15 An MRI image of the neck

An MRI instrument is especially useful for visualizing soft tissue. In 2002, 60 million MRI procedures were performed. The 2003 Nobel Prize in Physiology or Medicine was awarded to chemist Paul C. Lauterbur and physicist Sir Peter Mansfield for their contributions in developing magnetic resonance imaging.



A: Spinal cord compression from a herniated disc
B: Spinal cord (would not be visualized with conventional X-rays)