

Chapter 2

Representative Carbon Compounds: Functional Groups, Intermolecular Forces and Infrared (IR) Spectroscopy

◆ Carbon-carbon Covalent Bonds

- Carbon forms strong covalent bonds to other carbons and to other elements such as hydrogen, oxygen, nitrogen and sulfur
 - This accounts for the vast variety of organic compounds possible
- Organic compounds are grouped into functional group families
 - A *functional group* is a specific grouping of atoms (e.g. carbon-carbon double bonds are in the family of alkenes)
 - An instrumental technique called infrared (IR) spectroscopy is used to determine the presence of specific functional groups

◆ Hydrocarbons: Representative Alkanes, Alkenes, Alkynes, and Aromatic Compounds

→ Hydrocarbons contain only carbon and hydrogen atoms

→ Subgroups of Hydrocarbons:

- ⌘ Alkanes contain only carbon-carbon single bonds
- ⌘ Alkenes contain one or more carbon-carbon double bonds
- ⌘ Alkynes contain one or more carbon-carbon triple bonds
- ⌘ Aromatic hydrocarbons contain benzene-like stable structures (discussed later)

→ Saturated hydrocarbons: contain only carbon-carbon single bonds e.g. alkanes

→ Unsaturated hydrocarbons: contain double or triple carbon-carbon bonds e.g. alkene, alkynes, aromatics

- ⌘ Contain fewer than maximum number of hydrogens per carbon
- ⌘ Capable of reacting with H_2 to become saturated

◆ Representative Hydrocarbons

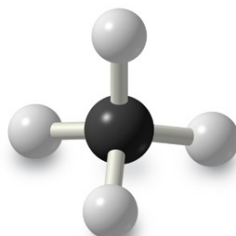
● Alkanes

→ Principle sources of alkanes are natural gas and petroleum

- ⌘ Smaller alkanes (C_1 to C_4) are gases at room temperature

→ Methane is

- ⌘ A component of the atmosphere of many planets
- ⌘ Major component of natural gas
- ⌘ Produced by primitive organisms called methanogens found in mud, sewage and cows' stomachs

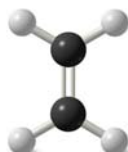


Methane

- Alkenes

→ Ethene (ethylene) is a major industrial feedstock

⌘ Used in the production of ethanol, ethylene oxide and the polymer polyethylene



Ethene

→ Propene (propylene) is also very important in industry

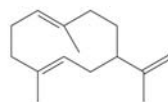
⌘ Molecular formula C_3H_6

⌘ Used to make the polymer polypropylene and is the starting material for acetone

→ Many alkenes occur naturally



β -Pinene
(a component of turpentine)



An aphid alarm pheromone

Chapter 2

5

- Alkynes

→ Ethyne (acetylene) is used in welding torches because it burns at high temperature



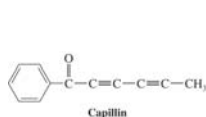
Ethyne

→ Many alkynes are of biological interest

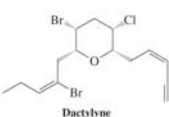
⌘ Capillin is an antifungal agent found naturally

⌘ Dactylone is a marine natural product

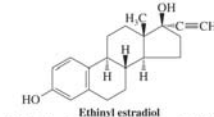
⌘ Ethinyl estradiol is a synthetic estrogen used in oral contraceptives



Capillin



Dactylone



Ethinyl estradiol
[17 α -ethynyl-1,3,5(10)-estratriene-3,17 β -diol]

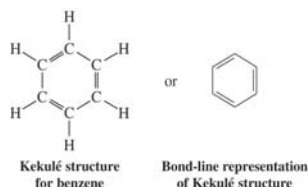
Chapter 2

6

- **Benzene: A Representative Hydrocarbon**

→ Benzene is the prototypical aromatic compound

⌘ The Kekulé structure (named after August Kekulé who formulated it) is a six-membered ring with alternating double and single bonds



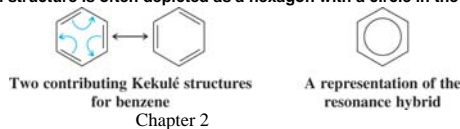
→ Benzene does not actually have discrete single and double carbon-carbon bonds

⌘ All carbon-carbon bonds are exactly equal in length (1.38 Å)

⌘ This is between the length of a carbon-carbon single bond and a carbon-carbon double bond

→ Resonance theory explains this by suggesting there are two resonance hybrids that contribute equally to the real structure

⌘ The real structure is often depicted as a hexagon with a circle in the middle



Chapter 2

7

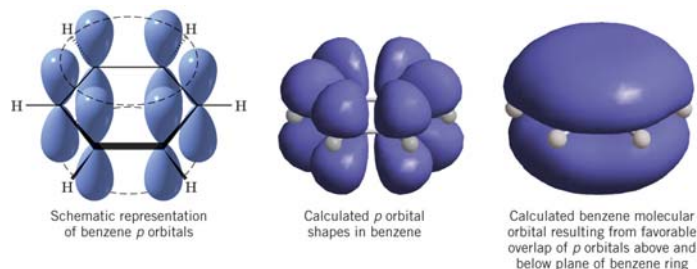
- **Molecular orbital theory explains the equal bond lengths of benzene by suggesting there is a continuous overlap of p orbitals over the entire ring**

→ All carbons in benzene are sp^2 hybridized

⌘ Each carbon also has a p orbital

→ Each p orbital does not just overlap with one adjacent p but overlaps with p orbitals on either side to give a continuous bonding molecular orbital that encompasses all 6 carbons

→ All 6 π electrons are therefore *delocalized* over the entire ring and this results in the equivalence of all of the carbon-carbon bonds



Chapter 2

8

◆ Polar Covalent Bonds

- Polar covalent bonds occur when a covalent bond is formed between two atoms of differing electronegativities

→ The more electronegative atom draws electron density closer to itself

→ The more electronegative atom develops a partial negative charge (δ^-) and the less electronegative atom develops a partial positive charge (δ^+)

→ A bond which is polarized is a dipole and has a dipole moment

→ The direction of the dipole can be indicated by a dipole arrow

‡ The arrow head is the negative end of a dipole, the crossed end is the positive end

(positive end) \longleftrightarrow (negative end)

- Example: the molecule HCl

→ The more electronegative chlorine draws electron density away from the hydrogen

‡ Chlorine develops a partial negative charge



- The dipole moment of a molecule can be measured experimentally

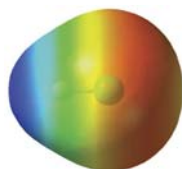
→ It is the product of the magnitude of the charges (in electrostatic units: esu) and the distance between the charges (in cm)

→ The actual unit of measurement is a Debye (D) which is equivalent to 1×10^{-18} esu cm

Dipole moment = charge (in esu) \times distance (in cm)

$$\mu = e \times d$$

- **A map of electrostatic potential (MEP) is a way to visualize distribution of charge in a molecule**
 - **Parts of the molecule which are red have relatively more electron density or are negative**
 - ⌘ These region would tend to attract positively charged species
 - **Parts of the molecule which are blue have relatively less electron density or are positive**
 - ⌘ These region would tend to attract negatively charged species
 - **The MEP is plotted at the van Der Waals surface of a molecule**
 - ⌘ This is the farthest extent of a molecule's electron cloud and therefore indicates the shape of the molecule
 - **The MEP of hydrogen chlorine clearly indicates that the negative charge is concentrated near chlorine**
 - ⌘ The overall shape of the molecule is also represented



Chapter 2

11

◆ Molecular Dipole

- In diatomic molecules a dipole exists if the two atoms are of different electronegativity
- In more complicated molecules the molecular dipole is the sum of the bond dipoles
- Some molecules with very polar bonds will have no net molecular dipole because the bond dipoles cancel out
 - ⌘ The center of positive charge and negative charge coincide in these molecules

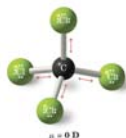
Formula	μ (D)	Formula	μ (D)
H ₂	0	CH ₄	0
Cl ₂	0	CH ₃ Cl	1.87
HF	1.91	CH ₂ Cl ₂	1.55
HCl	1.08	CHCl ₃	1.02
HBr	0.80	CCl ₄	0
HI	0.42	NH ₃	1.47
BF ₃	0	NF ₃	0.24
CO ₂	0	H ₂ O	1.85

Chapter 2

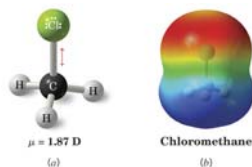
12

- **Examples**

→ In carbon tetrachloride the bond dipoles cancel and the overall molecular dipole is 0 Debye



→ In chloromethane the C-H bonds have only small dipoles but the C-Cl bond has a large dipole and the molecule is quite polar

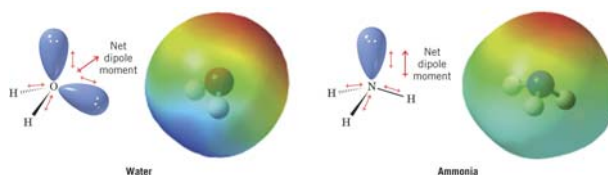


→ An unshared pair of electrons on atoms such as oxygen and nitrogen contribute a great deal to a dipole

⚡ Water and ammonia have very large net dipoles

Chapter 2

13



- **Some cis-trans isomers differ markedly in their dipole moment**

→ In trans 1,2-dichloroethene the two carbon-chlorine dipoles cancel out and the molecular dipole is 0 Debye

→ In the cis isomer the carbon-chlorine dipoles reinforce and there is a large molecular dipole

Compound	Melting Point (°C)	Boiling Point (°C)	Dipole Moment (D)
cis-1,2-Dichloroethene	-80	60	1.90
trans-1,2-Dichloroethene	-50	48	0
cis-1,2-Dibromoethene	-53	112.5	1.35
trans-1,2-Dibromoethene	-6	108	0

Chapter 2

14

◆ Functional Groups

→ Functional group families are characterized by the presence of a certain arrangement of atoms called a *functional group*

→ A functional group is the site of most chemical reactivity of a molecule

⌘ The functional group is responsible for many of the physical properties of a molecule

→ Alkanes do not have a functional groups

⌘ Carbon-carbon single bonds and carbon-hydrogen bonds are generally very unreactive

● Alkyl Groups and the Symbol R

→ Alkyl groups are obtained by removing a hydrogen from an alkane

→ Often more than one alkyl group can be obtained from an alkane by removal of different kinds of hydrogens

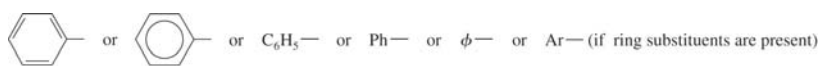
ALKANE	ALKYL GROUP	ABBREVIATION
CH ₄ Methane	CH ₃ — Methyl group	Me—
CH ₃ CH ₃ Ethane	CH ₃ CH ₂ — or C ₂ H ₅ — Ethyl group	Et—
CH ₃ CH ₂ CH ₃ Propane	CH ₃ CH ₂ CH ₂ — Propyl group	Pr—
CH ₃ CH ₂ CH ₃ Propane	CH ₃ CH(CH ₃)— or CH ₃ CH— Isopropyl group	<i>i</i> -Pr—

→ R is the symbol to represent a generic alkyl groups

⌘ The general formula for an alkane can be abbreviated R-H

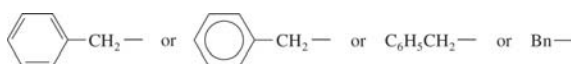
CH ₃ —	Methyl	} These and others can be designated by R.
CH ₃ CH ₂ —	Ethyl	
CH ₃ CH ₂ CH ₂ —	Propyl	
CH ₃ CH(CH ₃)—	Isopropyl	

→ A benzene ring with a hydrogen removed is called a *phenyl* and can be represented in various ways



Ways of representing a phenyl group

→ Toluene (methylbenzene) with its methyl hydrogen removed is called a *benzyl* group



Ways of representing a benzyl group

Chapter 2

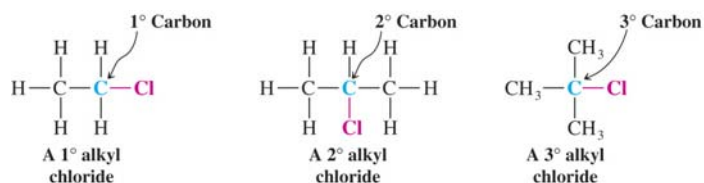
17

● Alkyl Halides

→ In alkyl halides, halogen (F, Cl, Br, I) replaces the hydrogen of an alkane

→ They are classified based on the carbon the halogen is attached to

- ⌘ If the carbon is attached to one other carbon that carbon is primary (1°) and the alkyl halide is also 1°
- ⌘ If the carbon is attached to two other carbons, that carbon is secondary (2°) and the alkyl halide is 2°
- ⌘ If the carbon is attached to three other carbons, the carbon is tertiary (3°) and the alkyl halide is 3°



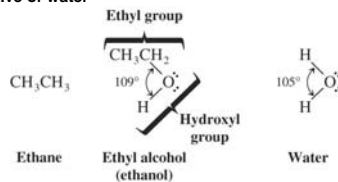
Chapter 2

18

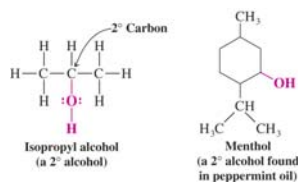
● Alcohols

→ In alcohols the hydrogen of the alkane is replaced by the hydroxyl (-OH) group

⌘ An alcohol can be viewed as either a hydroxyl derivative of an alkane or an alkyl derivative of water



→ Alcohols are also classified according to the carbon the hydroxyl is directly attached to



Chapter 2

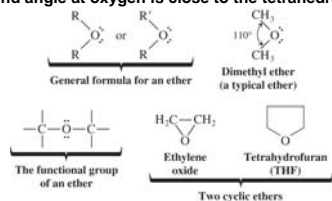
19

● Ethers

→ Ethers have the general formula R-O-R or R-O-R' where R' is different from R

⌘ These can be considered organic derivatives of water in which both hydrogens are replaced by organic groups

⌘ The bond angle at oxygen is close to the tetrahedral angle



● Amines

→ Amines are organic derivatives of ammonia

⌘ They are classified according to how many alkyl groups replace the hydrogens of ammonia

⌘ This is a different classification scheme than that used in alcohols



Chapter 2

20

- **Aldehydes and Ketones**

→ Both contain the carbonyl group

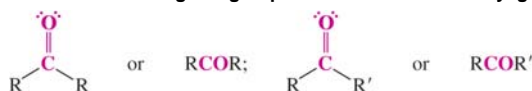


The carbonyl group

→ Aldehydes have at least one carbon attached to the carbonyl group

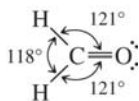


→ Ketones have two organic groups attached to the carbonyl group



→ The carbonyl carbon is sp^2 hybridized

It is trigonal planar and has bond angle about 120°



Chapter 2

21

- **Carboxylic Acids, Esters and Amides**

→ All these groups contain a carbonyl group bonded to an oxygen or nitrogen

→ Carboxylic Acids

Contain the carboxyl (carbonyl + hydroxyl) group



→ Esters

A carbonyl group is bonded to an alkoxy (OR') group



General formula for an ester



A specific ester called ethyl acetate

Chapter 2

22

→ Amide

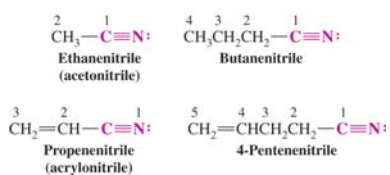
⌘ A carbonyl group is bonded to a nitrogen derived from ammonia or an amine



● Nitriles

→ An alkyl group is attached to a carbon triply bonded to a nitrogen

⌘ This functional group is called a cyano group



Chapter 2

23

Summary of Important Families of Organic Compounds

	Family						
	Alkane	Alkene	Alkyne	Aromatic	Haloalkane	Alcohol	Ether
Functional group	C—H and C—C bonds			Aromatic ring			
General formula	RH	RCH=CH ₂ RCH=CHR R ₂ C=CHR R ₂ C=CR ₂	RC≡CH RC≡CR	ArH	RX	ROH	ROR
Specific example	CH ₃ CH ₃	CH ₂ =CH ₂	HC≡CH		CH ₃ CH ₂ Cl	CH ₃ CH ₂ OH	CH ₃ OCH ₃
IUPAC name	Ethane	Ethene	Ethyne	Benzene	Chloroethane	Ethanol	Methoxymethane
Common name ^a	Ethane	Ethylene	Acetylene	Benzene	Ethyl chloride	Ethyl alcohol	Dimethyl ether

^aThese names are also accepted by the IUPAC.

Chapter 2

24

◆ Summary (cont.)

Family						
Amine	Aldehyde	Ketone	Carboxylic Acid	Ester	Amide	Nitrile
RNH ₂ R ₂ NH R ₃ N	RCH=O	R ₂ C=O	RCOOH	RCOR'	RC(=O)NH ₂ RC(=O)NHR' RC(=O)NR'R''	RC≡N
CH ₃ NH ₂	CH ₃ CHO	CH ₃ COCH ₃	CH ₃ COOH	CH ₃ COOCH ₃	CH ₃ CONH ₂	CH ₃ C≡N
Methanamine	Ethanal	Propanone	Ethanoic acid	Methyl ethanoate	Ethanamide	Ethanenitrile
Methylamine	Acetaldehyde	Acetone	Acetic acid	Methyl acetate	Acetamide	Acetonitrile

Chapter 2

25

◆ Physical Properties and Molecular Structure

- The strength of intermolecular forces (forces between molecules) determines the physical properties (*i.e.* melting point, boiling point and solubility) of a compound
- Stronger intermolecular forces result in high melting points and boiling points
 - ↳ More energy must be expended to overcome very strong forces between molecules
- The type of intermolecular forces important for a molecule are determined by its structure
- The physical properties of some representative compounds are shown on the next slide

Chapter 2

26

Compound	Structure	mp (°C)	bp (°C) (1 atm) ^a
Methane	CH ₄	-182.6	-162
Ethane	CH ₃ CH ₃	-183	-88.2
Ethene	CH ₂ =CH ₂	-169	-102
Ethyne	HC≡CH	-82	-84 subl
Chloromethane	CH ₃ Cl	-97	-23.7
Chloroethane	CH ₃ CH ₂ Cl	-138.7	13.1
Ethyl alcohol	CH ₃ CH ₂ OH	-115	78.5
Acetaldehyde	CH ₃ CHO	-121	20
Acetic acid	CH ₃ CO ₂ H	16.6	118
Sodium acetate	CH ₃ CO ₂ Na	324	dec
Ethylamine	CH ₃ CH ₂ NH ₂	-80	17
Diethyl ether	(CH ₃ CH ₂) ₂ O	-116	34.6
Ethyl acetate	CH ₃ CO ₂ CH ₂ CH ₃	-84	77

^aIn this table dec = decomposes and subl = sublimes.

Chapter 2

27

● Ion-Ion Forces

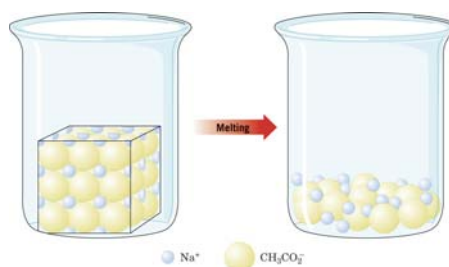
→ Ion-ion forces are between positively and negatively charged ions

→ These are very strong forces that hold a solid compound consisting of ions together in a crystalline lattice

‡ Melting points are high because a great deal of energy is required to break apart the crystalline lattice

→ Boiling points are so high that organic ions often decompose before they boil

→ Example: Sodium acetate



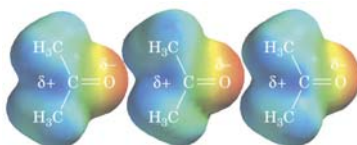
Chapter 2

28

- **Dipole-Dipole Forces**

- Dipole-dipole forces are between molecules with permanent dipoles

- ⌘ There is an interaction between $\delta+$ and $\delta-$ areas in each molecule; these are much weaker than ion-ion forces
- ⌘ Molecules align to maximize attraction of $\delta+$ and $\delta-$ parts of molecules
- ⌘ Example: acetone



Chapter 2

29

- **Hydrogen Bonds**

- Hydrogen bonds result from very strong dipole-dipole forces

- There is an interaction between hydrogens bonded to strongly electronegative atoms (O, N or F) and nonbonding electron pairs on other strongly electronegative atoms (O, N or F)



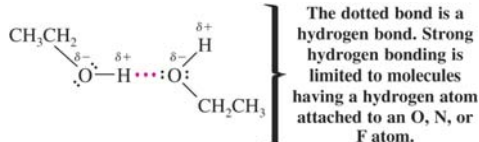
Chapter 2

30

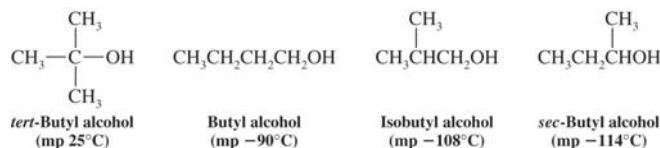
- **Example**

→ Ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) has a boiling point of $+78.5^\circ\text{C}$; its isomer methyl ether (CH_3OCH_3) has a boiling point of -24.9°C

⚡ Ethanol molecules are held together by hydrogen bonds whereas methyl ether molecules are held together only by weaker dipole-dipole interactions



→ A factor in melting points is that symmetrical molecules tend to pack better in the crystalline lattice and have higher melting points



Chapter 2

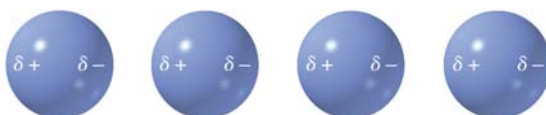
31

- **van der Waals Forces (London or Dispersion Forces)**

→ Van der Waals forces result when a temporary dipole in a molecule caused by a momentary shifting of electrons induces an opposite and also temporary dipole in an adjacent molecule

⚡ These temporary opposite dipoles cause a weak attraction between the two molecules

⚡ Molecules which rely only on van der Waals forces generally have low melting points and boiling points



Chapter 2

32

→ **Polarizability predicts the magnitude of van der Waals Interactions**

- ⌘ Polarizability is the ability of the electrons on an atom to respond to a changing electric field
- ⌘ Atoms with very loosely held electrons are more polarizable
- ⌘ Iodine atoms are more polarizable than fluorine atoms because the outer shell electrons are more loosely held
- ⌘ Atoms with unshared electrons are more polarizable (a halogen is more polarizable than an alkyl of similar size)

Molecule	Dipole Moment (D)	Attractive Energies (kJ mol ⁻¹)		Melting Point (°C)	Boiling Point (°C)
		Dipole–Dipole	van der Waals		
H ₂ O	1.85	36 ^a	8.8	0	100
NH ₃	1.47	14 ^a	15	-78	-33
HCl	1.08	3 ^a	17	-115	-85
HBr	0.80	0.8	22	-88	-67
HI	0.42	0.03	28	-51	-35

^aThese dipole–dipole attractions are called hydrogen bonds.

→ **All things being equal larger and heavier molecules have higher boiling points**

- ⌘ Larger molecules need more energy to escape the surface of the liquid
- ⌘ Larger organic molecules tend to have more surface area in contact with each other and so have stronger van der Waals interactions
- ⌘ Methane (CH₄) has a boiling point of -162°C whereas ethane (C₂H₆) has a boiling point of -88.2°C

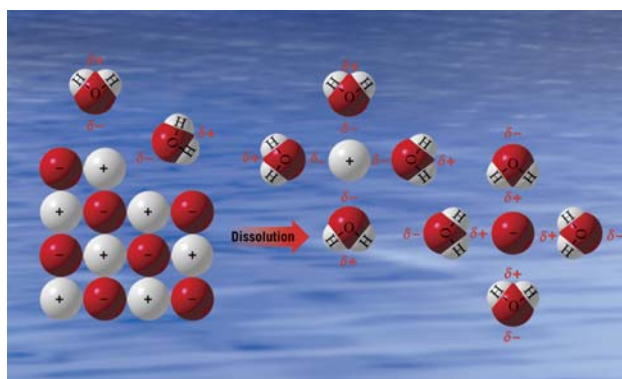
Chapter 2

33

● **Solubilities**

→ **Water dissolves ionic solids by forming strong dipole-ion interactions**

- ⌘ These dipole-ion interactions are powerful enough to overcome lattice energy and interionic interactions in the solid

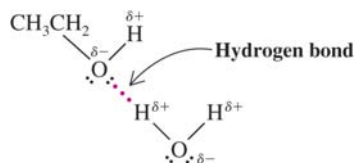


Chapter 2

34

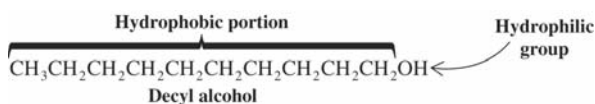
→ Generally like dissolves like

- ⌘ Polar solvents tend to dissolve polar solids or polar liquids
- ⌘ Methanol (a water-like molecule) dissolves in water in all proportions and interacts using hydrogen-bonding to the water



→ A large alkyl group can overwhelm the ability of the polar group to solubilize a molecule in water

- ⌘ Decyl alcohol is only slightly soluble in water
- ⌘ The large alkyl portion is hydrophobic (“water hating”) and overwhelms the capacity of the hydrophilic (“water loving”) hydroxyl



Chapter 2

35

→ Generally one hydrophilic group (e.g. hydroxyl) can make a compound with 3 carbons completely soluble in water

- ⌘ One hydrophilic group can make a 5 carbon compound at least partially soluble
- ⌘ A compound is water soluble if at least 3g of it will dissolve in 100 mL water

◆ Summary of Attractive Electric Forces

Electric Force	Relative Strength	Type	Example
Cation–anion (in a crystal)	Very strong	$\oplus \ominus$	Lithium fluoride crystal lattice
Covalent bonds	Strong (140–523 kJ mol ⁻¹)	Shared electron pairs	H–H (436 kJ mol ⁻¹) CH ₃ –CH ₃ (378 kJ mol ⁻¹) I–I (151 kJ mol ⁻¹)
Ion–dipole	Moderate		Na ⁺ in water (see Fig. 2.9)
Dipole–dipole (including hydrogen bonds)	Moderate to weak (4–38 kJ mol ⁻¹)	$\delta^- \cdots \delta^+$ and	
van der Waals	Variable	Transient dipole	Interactions between methane molecules

Chapter 2

36

◆ Infrared Spectroscopy: An Instrumental Method for Detecting Functional Groups

- Electromagnetic radiation in the infrared (IR) frequency range is absorbed by a molecule at certain characteristic frequencies
 - Energy is absorbed by the bonds in the molecule and they vibrate faster
 - The bonds behave like tiny springs connecting the atoms
 - ⌘ The bonds can absorb energy and vibrate faster only when the added energy is of a particular resonant frequency
 - The frequencies of absorption are very characteristic of the type of bonds contained in the sample molecule
 - The type of bonds present are directly related to the functional groups present
 - A plot of these absorbed frequencies is called an IR spectrum

Chapter 2

37

● Infrared Spectrometer

- An infrared spectrometer detects the frequencies absorbed by the sample molecule
- Light of all the various IR frequencies is transmitted to the molecule and the frequencies absorbed are recorded
- The absorption frequencies are specified as wavenumbers in units of reciprocal centimeters (cm^{-1})
 - ⌘ Alternatively the wavelength (λ) in units of microns (μm) can be specified

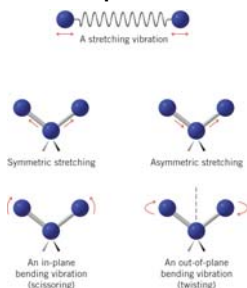
$$\bar{\nu} = \frac{1}{\lambda} \quad (\text{with } \lambda \text{ in cm}) \quad \text{or} \quad \bar{\nu} = \frac{10,000}{\lambda} \quad (\text{with } \lambda \text{ in } \mu\text{m})$$

- The spectrum is a plot of frequency on the horizontal axis versus strength of absorption on the vertical axis

Chapter 2

38

→ There are different types of stretching and bending vibrations induced by the absorption of infrared energy



→ The actual relative frequency of vibration can be predicted

⌘ Bonds with lighter atoms vibrate faster than those with heavier atoms

GROUP	BOND	FREQUENCY RANGE (CM ⁻¹)
Alkyl	C—H	2853–2962
Alcohol	O—H	3590–3650
Amine	N—H	3300–3500

Chapter 2

39

→ Triple bonds (which are stiffer and stronger) vibrate at higher frequencies than double bonds

⌘ Double bonds in turn vibrate at higher frequencies than single bonds

BOND	FREQUENCY RANGE (CM ⁻¹)
C≡C	2100–2260
C≡N	2220–2260
C=C	1620–1680
C=O	1630–1780

→ The IR spectrum of a molecule usually contains many peaks

- ⌘ These peaks are due to the various types of vibrations available to each of the different bonds
- ⌘ Additional peaks result from overtone (harmonic) peaks which are weaker and of lower frequency
- ⌘ The IR is a "fingerprint" of the molecule because of the unique and large number of peaks seen for a particular molecule

Chapter 2

40

Group	Frequency Range (cm ⁻¹)	Intensity*
A. Alkyl		
C-H (stretching)	2853-2962	(m-s)
Isopropyl, -CH(CH ₃) ₂	1380-1385	(s)
tert-Butyl, -C(CH ₃) ₃	and 1365-1370	(s)
	and 1385-1395	(m)
	and ~1365	(s)
B. Alkenyl		
C-H (stretching)	3010-3095	(m)
C=C (stretching)	1620-1680	(v)
R-CH=CH ₂	965-1000	(s)
R ₂ C=CH ₂	and 905-920	(s)
	and 880-900	(s)
(out-of plane C-H bendings)		
cis-RCH=CHR	675-730	(s)
trans-RCH=CHR	960-975	(s)
C. Alkynyl		
≡C-H (stretching)	~3300	(s)
C≡C (stretching)	2100-2260	(v)
D. Aromatic		
Ar-H (stretching)	~3030	(v)
Aromatic substitution type (C-H out-of plane bendings)		
Monosubstituted	690-710	(very s)
o-Disubstituted	and 730-770	(very s)
m-Disubstituted	735-770	(s)
	690-725	(s)
p-Disubstituted	and 750-810	(very s)
	800-860	(very s)
E. Alcohols, Phenols, and Carboxylic Acids		
O-H (stretching)	3590-3650	(sharp, v)
Alcohols, phenols (dilute solutions)	3200-3550	(broad, s)
Alcohols, phenols (hydrogen bonded)	2500-3000	(broad, v)
Carboxylic acids (hydrogen bonded)		
F. Aldehydes, Ketones, Esters, and Carboxylic Acids		
C=O (stretching)	1630-1780	(s)
Aldehydes	1690-1740	(s)
Ketones	1680-1750	(s)
Esters	1735-1750	(s)
Carboxylic acids	1710-1780	(s)
Amides	1630-1690	(s)
G. Amines		
N-H	3300-3500	(m)
H. Nitriles		
C≡N	2220-2260	(m)

*Abbreviations: s = strong, m = medium, w = weak, v = variable, ~ = approximately.

Chapter 2

41

◆ Interpreting IR Spectra

→ Generally only certain peaks are interpreted in the IR

⌘ Those peaks that are large and above 1400 cm⁻¹ are most valuable

● Hydrocarbons

→ The C-H stretching regions from 2800-3300 cm⁻¹ is characteristic of the type of carbon the hydrogen is attached to

→ C-H bonds where the carbon has more s character are shorter, stronger and stiffer and thus vibrate at higher frequency

⌘ C-H bonds at sp centers appear at 3000-3100 cm⁻¹

⌘ C-H bonds at sp² centers appear at about 3080 cm⁻¹

⌘ C-H bonds at sp³ centers appear at about 2800-3000 cm⁻¹

→ C-C bond stretching frequencies are only useful for multiple bonds

⌘ C-C double bonds give peaks at 1620-1680 cm⁻¹

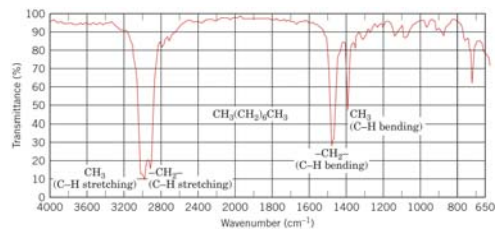
⌘ C-C triple bonds give peaks at 2100-2260 cm⁻¹

⌘ These peaks are absent in symmetrical double and triple bonds

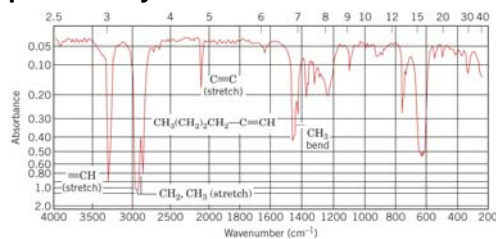
Chapter 2

42

- Example: octane



- Example: 1-hexyne

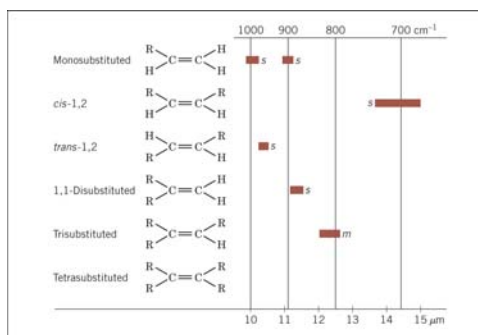


Chapter 2

43

- Alkenes

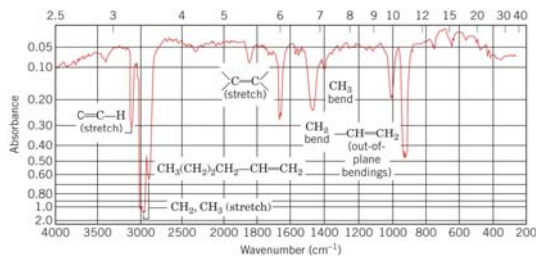
→ The C-H bending vibration peaks located at 600-1000 cm^{-1} can be used to determine the substitution pattern of the double bond



Chapter 2

44

- Example: 1-hexene



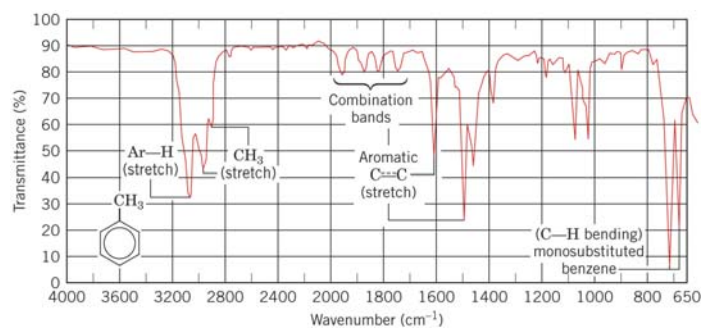
Chapter 2

45

- Aromatic Compounds

→ The C-C bond stretching gives a set of characteristic sharp peaks between 1450-1600 cm⁻¹

→ Example: Methyl benzene



Chapter 2

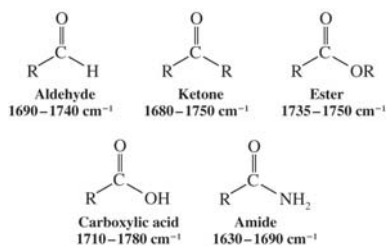
46

◆ Other Functional Groups

● Carbonyl Functional Groups

→ Generally the carbonyl group gives a strong peak which occurs at $1630-1780\text{ cm}^{-1}$

⌘ The exact location depends on the actual functional group present



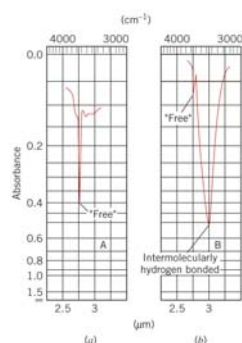
Chapter 2

47

● Alcohols and Phenols

→ The O-H stretching absorption is very characteristic

- ⌘ In very dilute solutions, hydrogen bonding is absent and there is a very sharp peak at $3590-3650\text{ cm}^{-1}$
- ⌘ In more concentrated solutions, the hydroxyl groups hydrogen bond to each other and a very broad and large peak occurs at $3200-3550\text{ cm}^{-1}$
- ⌘ A phenol has a hydroxyl group directly bonded to an aromatic ring



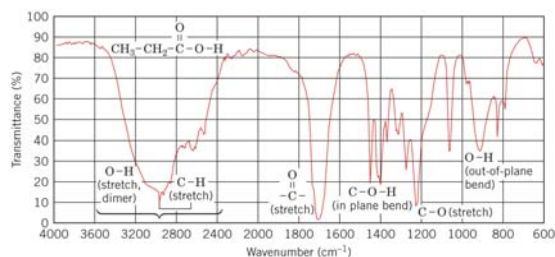
Chapter 2

48

Carboxylic Acids

- The carbonyl peak at $1710\text{-}1780\text{ cm}^{-1}$ is very characteristic
- The presence of both carbonyl and O-H stretching peaks is a good proof of the presence of a carboxylic acid

- Example: propanic acid



Chapter 2

49

- Amines

- Very dilute solution of 1° and 2° amines give sharp peaks at $3300\text{-}3500\text{ cm}^{-1}$ for the N-H stretching
 - ‡ 1° amines give two peaks and 2° amines give one peak
 - ‡ 3° have no N-H bonds and do not absorb in this region
- More concentrated solutions of amines have broader peaks
- Amides have amine N-H stretching peaks and a carbonyl peak

Chapter 2

50