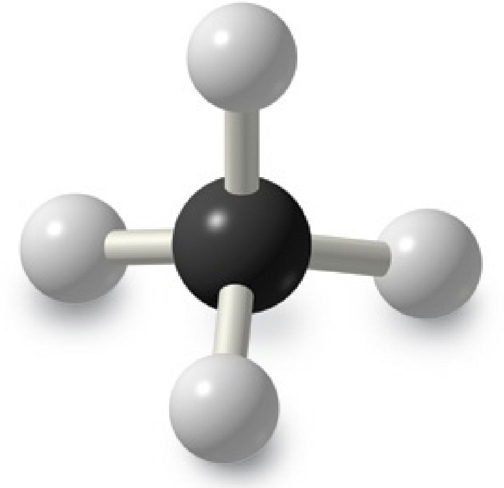
Representative Carbon Compounds Functional Groups, Intermolecular Forces and Infrared (IR) Spectroscopy

- **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**

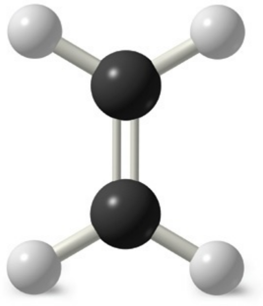
- **Hydrocarbons: Representative Alkanes, Alkenes Alkynes, and Aromatic Compounds**
  - **Hydrocarbons contain only carbon and hydrogen atoms**
  - **Subgroups of Hydrocarbons:**
    - **Alkanes contain only carbon-carbon single bonds**
    - **Alkenes contain one or more carbon-carbon double bonds**
    - **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

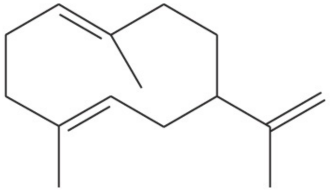
- **Alkenes**
  - **Ethene (ethylene) is a major industrial feedstock**
    - **Used in the production of ethanol, ethylene oxide and the polymer polyethylene**



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)

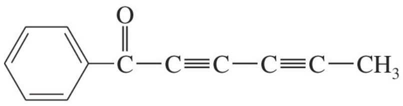


An aphid alarm pheromone

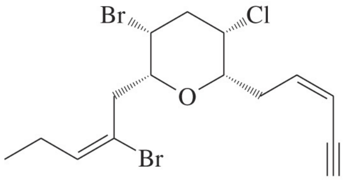
- **Alkynes**
  - **Ethyne (acetylene) is used in welding torches because it burns at high temperature**

Ethyne

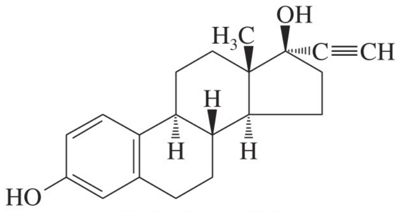
  - **Many alkynes are of biological interest**
    - **Capillin is an antifungal agent found naturally**
    - **Dactylyne is a marine natural product**
    - **Ethinyl estradiol is a synthetic estrogen used in oral contraceptives**



Capillin



Dactylyne

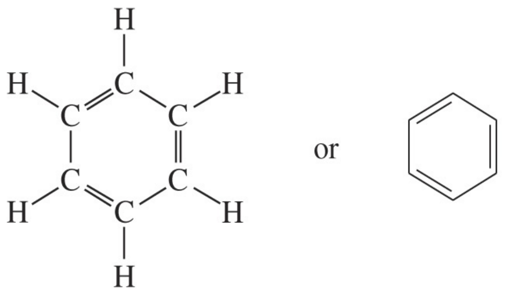


Ethinyl estradiol

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

Benzene: A Representative Hydrocarbon

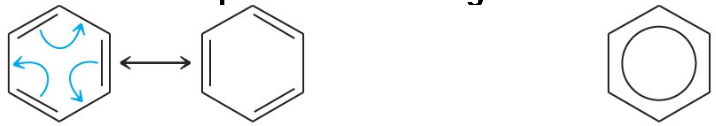
- Benzene is the prototypical aromatic compound
  - The Kekulé structure (named after August Kekulé who formulated it) is a six-membered ring with alternating double and single bonds



Kekulé structure for benzene

Bond-line representation of Kekulé structure

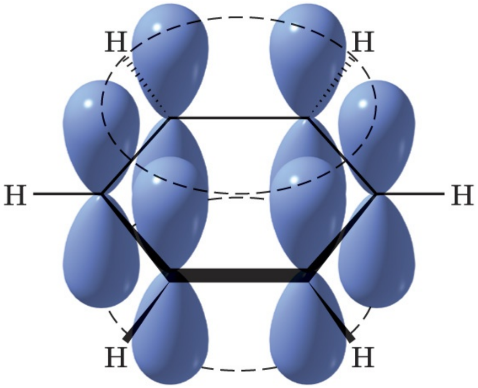
- Benzene does not actually have discreet single and double carbon-carbon bonds
  - All carbon-carbon bonds are exactly equal in length (1.38 Å)
  - This is between the length of a carbon-carbon single bond and a carbon-carbon double bond
- Resonance theory explains this by suggesting there are two resonance hybrids that contribute equally to the real structure
  - The real structure is often depicted as a hexagon with a circle in the middle



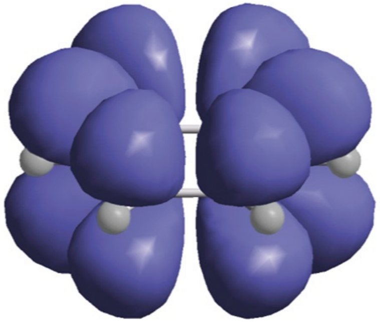
Two contributing Kekulé structures for benzene

A representation of the resonance hybrid

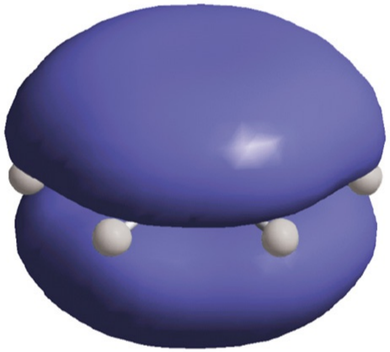
- **Molecular orbital theory explains the equal bond lengths of benzene by suggesting there in a continuous overlap of *p* orbitals over the entire ring**
  - **All carbons in benzene are *sp*^{2} hybridized**
    - **Each carbon also has a *p* orbital**
  - **Each *p* orbital does not just overlap with 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**



Schematic representation of benzene *p* orbitals



Calculated *p* orbital shapes in benzene



Calculated benzene molecular orbital resulting from favorable overlap of *p* orbitals above and below plane of benzene ring

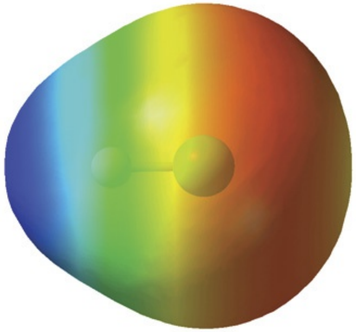
- **Polar Covalent Bonds**
  - **Polar covalent bonds occur when a covalent bond is formed between two atoms of differing electronegativities**
    - **The more electronegative atom draws electron density closer to itself**
    - **The more electronegative atom develops a partial negative charge (δ-) 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) ⟼ (negative end)

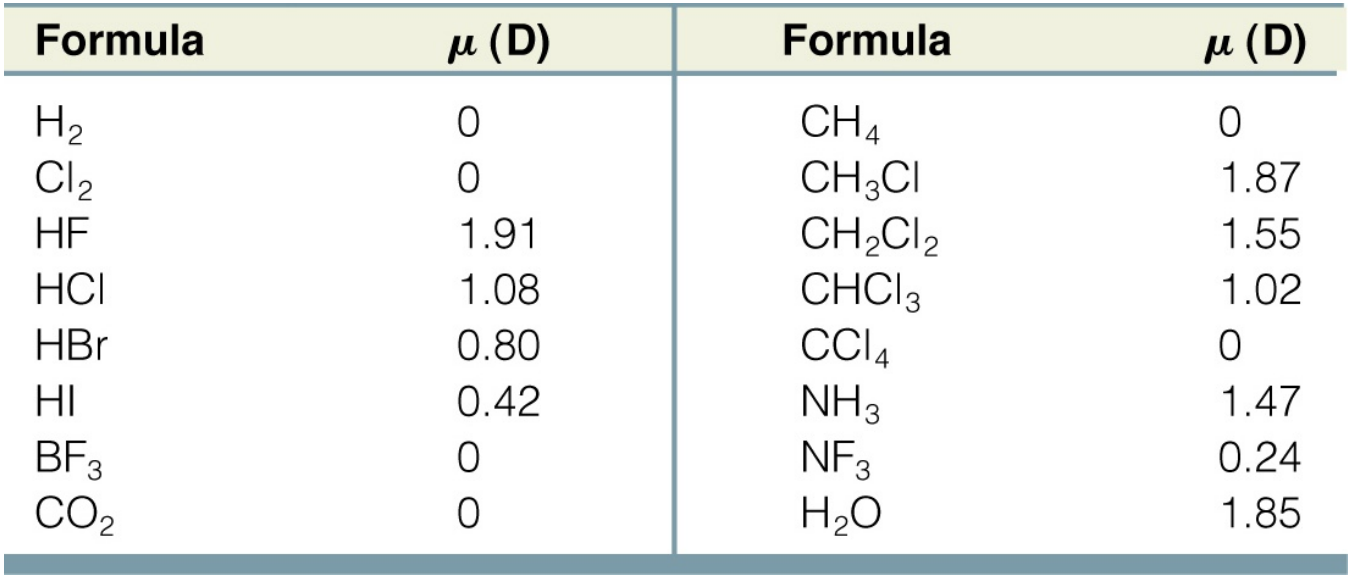
- **Example: the molecule HCl**
  - **The more electronegative chlorine draws electron density away from the hydrogen**
    - **Chlorine develops a partial negative charge**

- **The dipole moment of a molecule can be measured experimentally**

- 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

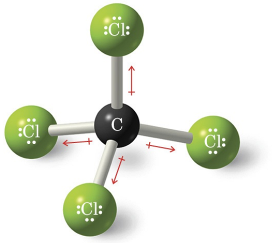


- **Molecular Dipole**
  - In diatomic molecules a dipole exists if the two atoms are of different electronegativity
  - In more complicated molecules the molecular dipole is the sum of the bond dipoles
  - Some molecules with very polar bonds will have no net molecular dipole because the bond dipoles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



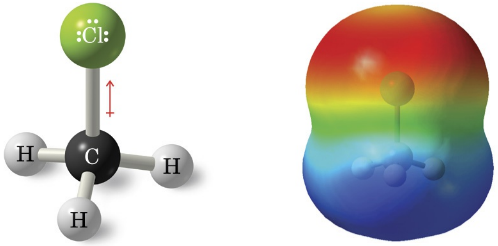
Formula	μ (D)	Formula	μ (D)
H_2	0	CH_4	0
Cl_2	0	CH_3Cl	1.87
HF	1.91	CH_2Cl_2	1.55
HCl	1.08	$CHCl_3$	1.02
HBr	0.80	CCl_4	0
HI	0.42	NH_3	1.47
BF_3	0	NF_3	0.24
CO_2	0	H_2O	1.85

- **Examples**
  - **In carbon tetrachloride the bond dipoles cancel and the overall molecular dipole is 0 Debye**



$\mu = 0$ D

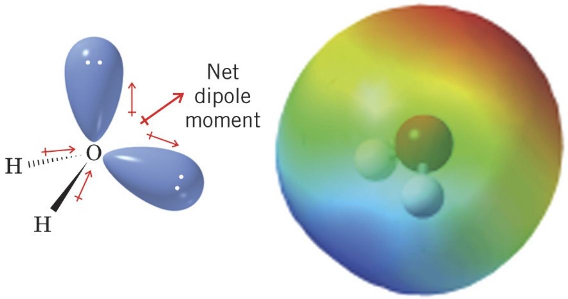
  - **In chloromethane the C-H bonds have only small dipoles but the C-Cl bond has a large dipole and the molecule is quite polar**



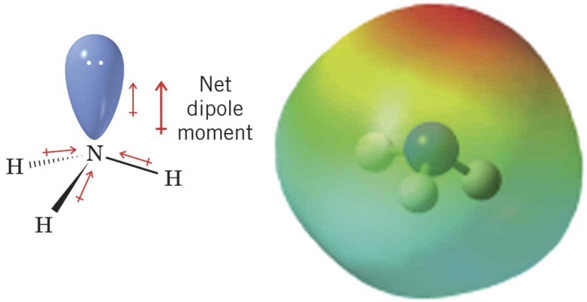
$\mu = 1.87$ D — Chloromethane

(a) (b)

  - **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**



Water



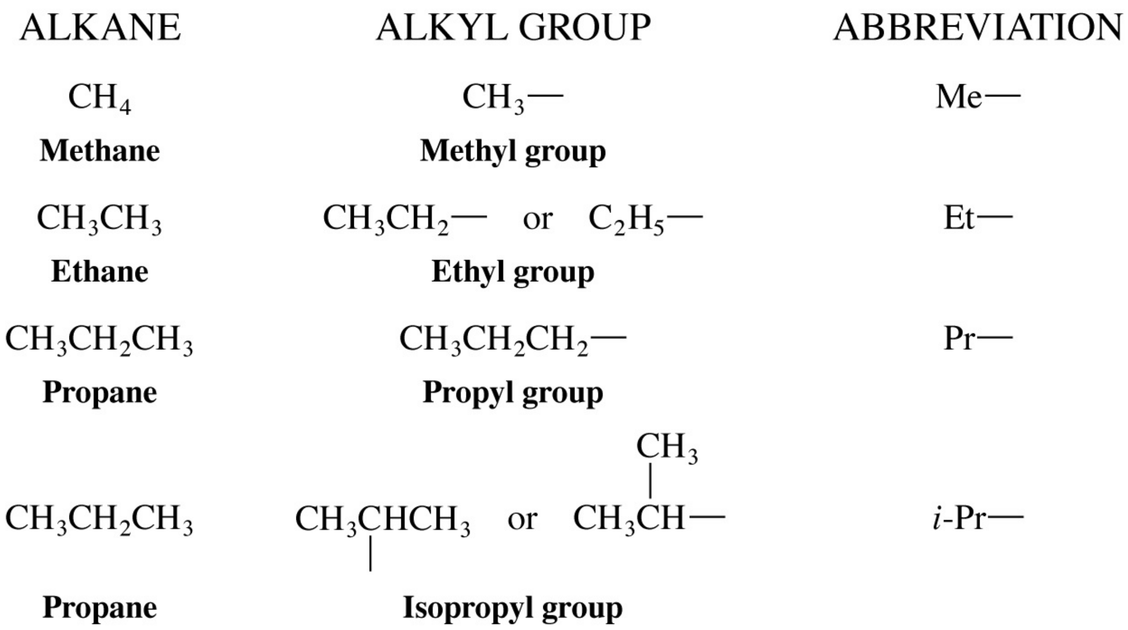
Ammonia

- **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

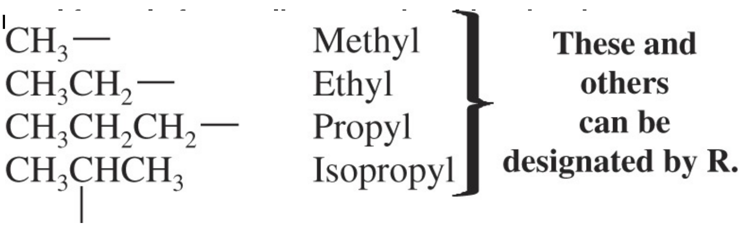
- **Functional Groups**
  - **Functional group families are characterized by the presence of a certain arrangement of atoms called a *functional group***
  - **A functional group is the site of most chemical reactivity of a molecule**
    - **The functional group is responsible for many of the physical 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_3CH_3 **Ethane**	$CH_3CH_2—$ or $C_2H_5—$ **Ethyl group**	Et—
$CH_3CH_2CH_3$ **Propane**	$CH_3CH_2CH_2—$ **Propyl group**	Pr—
$CH_3CH_2CH_3$ **Propane**	$CH_3\underset{\vert}{C}HCH_3$ or $CH_3\overset{CH_3}{\overset{\vert}{C}}H—$ **Isopropyl group**	*i*-Pr—

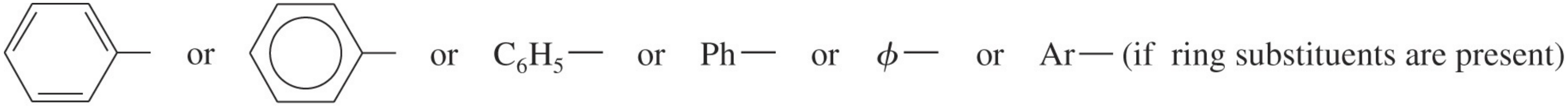
  - **R is the symbol to represent a generic alkyl groups**
    - **The ge**



$CH_3—$ Methyl
$CH_3CH_2—$ Ethyl
$CH_3CH_2CH_2—$ Propyl
$CH_3\underset{\vert}{C}HCH_3$ Isopropyl

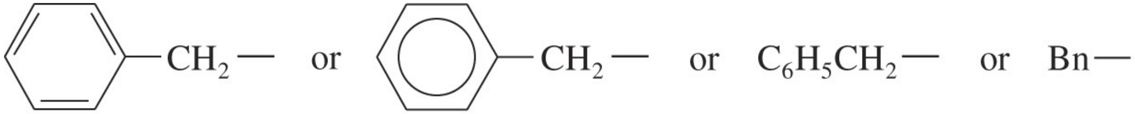
These and others can be designated by R.

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



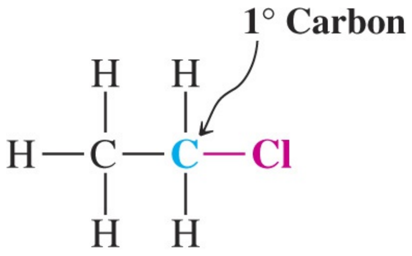
Ways of representing a phenyl group

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

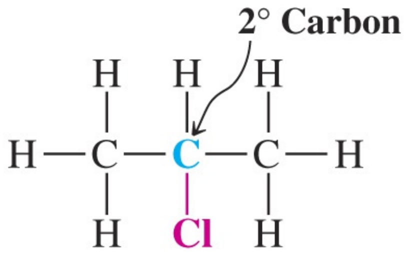


Ways of representing a benzyl group

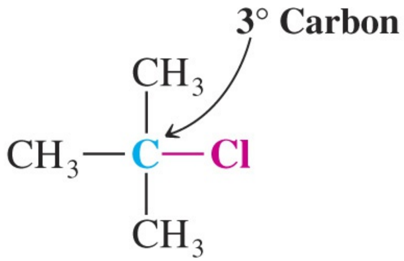
- **Alkyl Halides**
  - **In alkyl halides, halogen (F, Cl, Br, I) replaces the hydrogen of an alkane**
  - **They are classified based on the carbon the halogen is attached to**
    - **If the carbon is attached to one other carbon that carbon is primary (1^{o}) and the alkyl halide is also 1^{o}**
    - **If the carbon is attached to two other carbons, that carbon is secondary (2^{o}) and the alkyl halide is 2^{o}**
    - **If the carbon is attached to three other carbons, the carbon is tertiary (3^{o}) and the alkyl halide is 3^{o}**



A 1° alkyl chloride

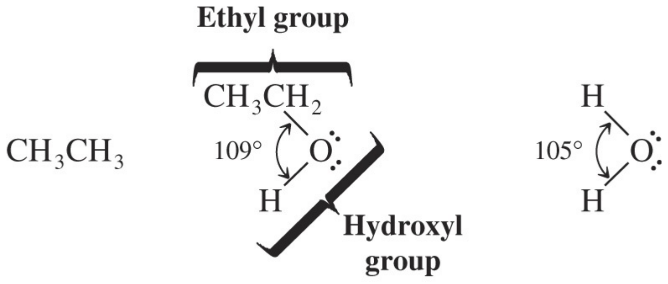


A 2° alkyl chloride



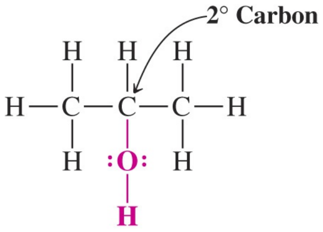
A 3° alkyl chloride

- **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**

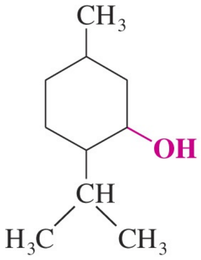


Ethane **Ethyl alcohol (ethanol)** **Water**

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

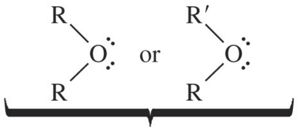


Isopropyl alcohol
(a 2° alcohol)

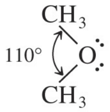


Menthol
(a 2° alcohol found in peppermint oil)

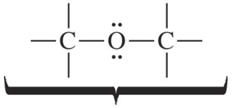
- **Ethers**
  - **Ethers have the general formula R-O-R or R-O-R’ where R’ is different from R**
    - **These can be considered organic derivatives of water in which both hydrogens are replaced by organic groups**
    - **The bond angle at oxygen is close to the tetrahedral angle**



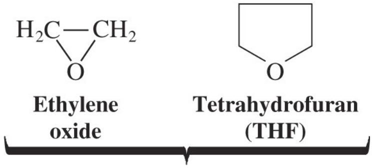
General formula for an ether



Dimethyl ether
(a typical ether)



The functional group
of an ether

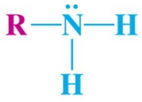


Ethylene
oxide

Tetrahydrofuran
(THF)

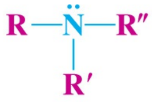
Two cyclic ethers

- **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**



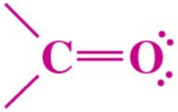
A primary (1°)
amine

A secondary (2°)
amine



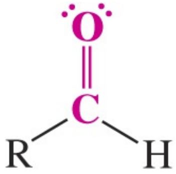
A tertiary (3°)
amine

- **Aldehydes and Ketones**
  - **Both contain the carbonyl group**



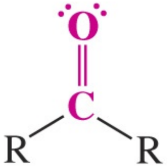
The carbonyl group

  - **Aldehydes have at least one carbon attached to the carbonyl group**

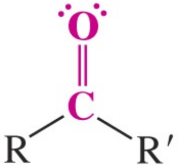


or RCHO R may also be H

  - **Ketones have two organic groups attached to the carbonyl group**

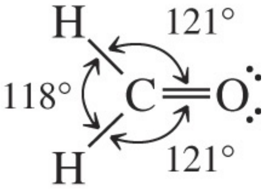


or RCOR;

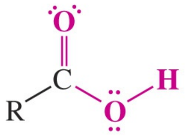


or RCOR′

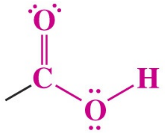
  - **The carbonyl carbon is *sp*^{2} hybridized**
    - **It is trigonal planar and has bond angle about 120^o**



- **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**

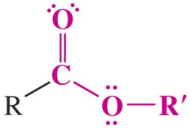

or RCO_2H or $RCOOH$

A carboxylic acid

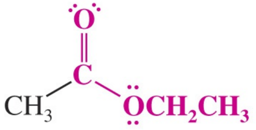

or $—CO_2H$ or $—COOH$

The carboxyl group

-
  - **Esters**
    - **A carbonyl group is bonded to an alkoxyl (OR’) group**

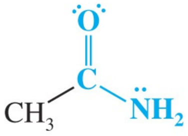

or RCO_2R' or $RCOOR'$

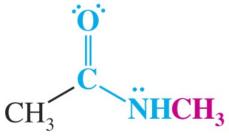
General formula for an ester

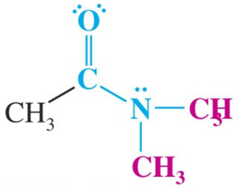

or $CH_3CO_2CH_2CH_3$ or $CH_3COOCH_2CH_3$

A specific ester called ethyl acetate

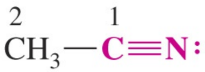
- **Amide**
  - A carbonyl group is bonded to a nitrogen derived from ammonia or an amine


Acetamide

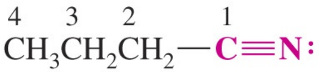

N-Methylacetamide


N,N-Dimethylacetamide

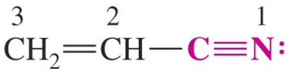
- Nitriles
  - An alkyl group is attached to a carbon triply bonded to a nitrogen
    - This functional group is called a cyano group


$\overset{2}{CH_3}-\overset{1}{C}\equiv N:$

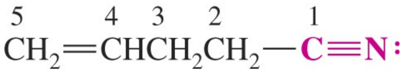
Ethanenitrile
(acetonitrile)


$\overset{4}{CH_3}\overset{3}{CH_2}\overset{2}{CH_2}-\overset{1}{C}\equiv N:$

Butanenitrile

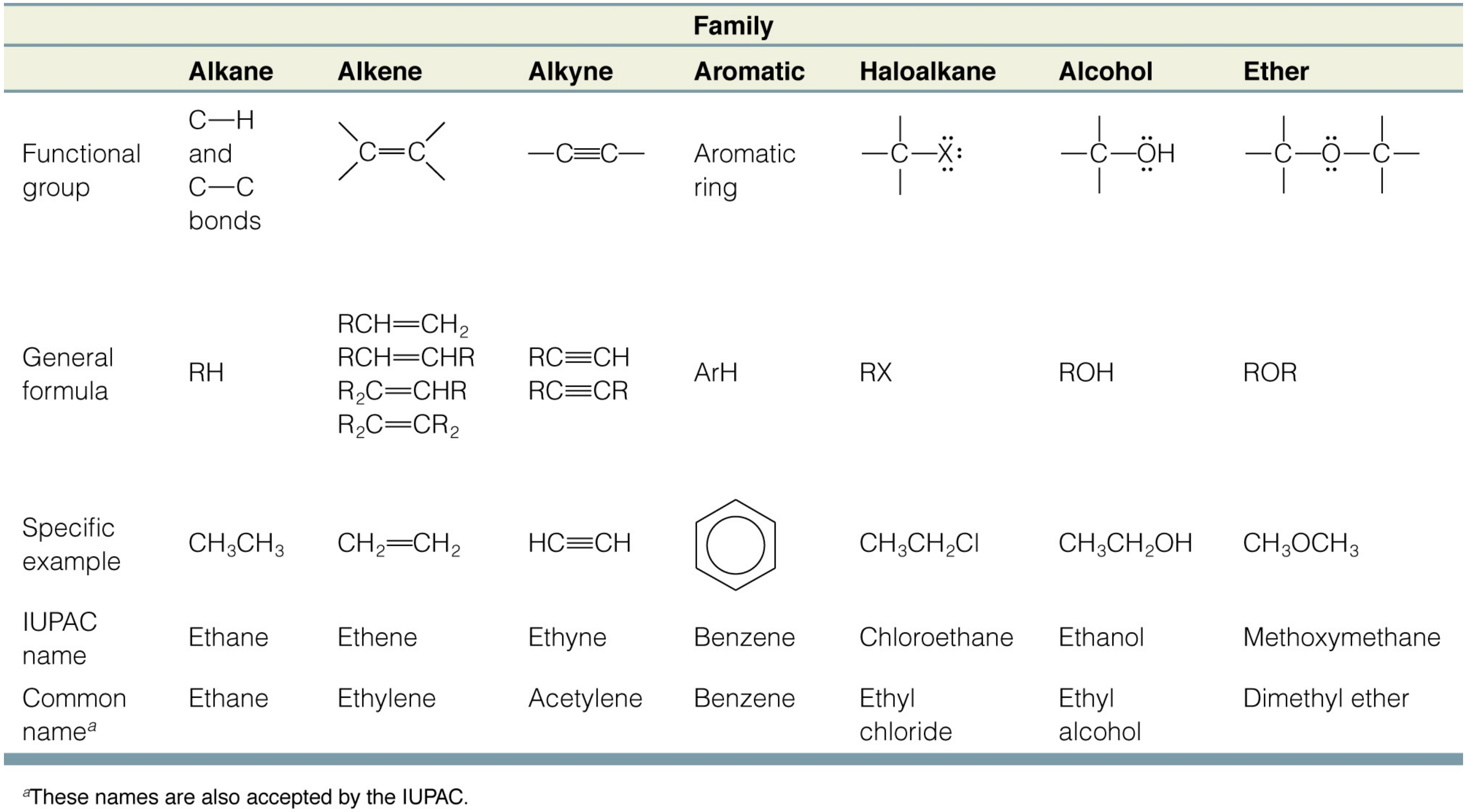

$\overset{3}{CH_2}=\overset{2}{CH}-\overset{1}{C}\equiv N:$

Propenenitrile
(acrylonitrile)


$\overset{5}{CH_2}=\overset{4}{CH}\overset{3}{CH_2}\overset{2}{CH_2}-\overset{1}{C}\equiv N:$

4-Pentenenitrile

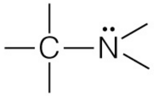
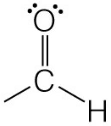
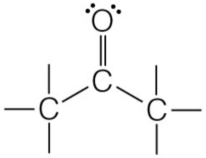
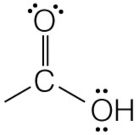
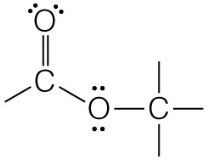
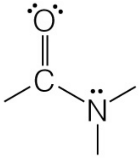
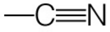
Summary of Important Families of Organic Compounds



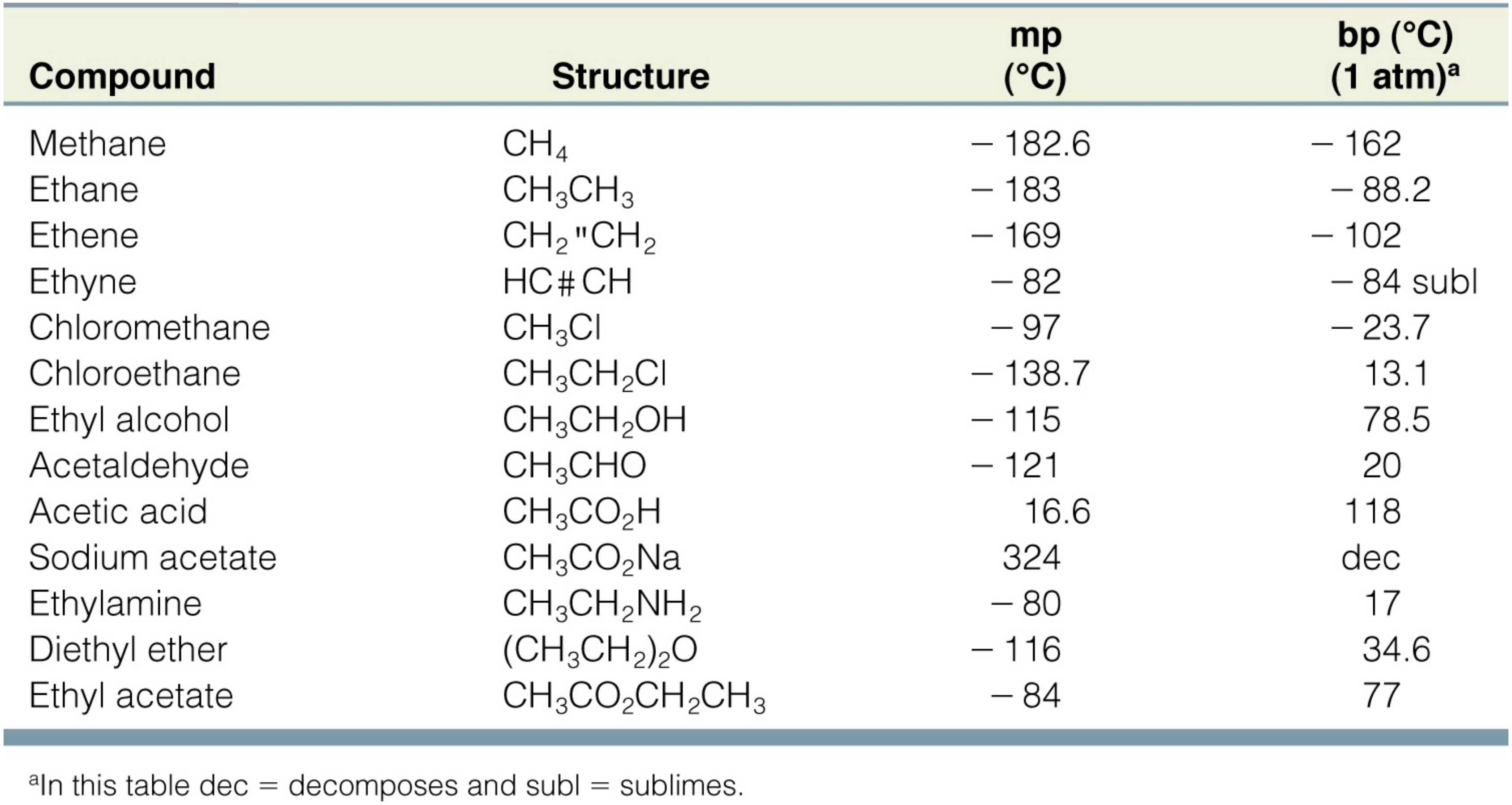
	Family						
	Alkane	**Alkene**	**Alkyne**	**Aromatic**	**Haloalkane**	**Alcohol**	**Ether**
Functional group	C—H and C—C bonds	$\gt C=C \lt$	$-C\equiv C-$	Aromatic ring	$-\overset{\vert}{\underset{\vert}{C}}-\ddot{\underset{\cdot\cdot}{X}}:$	$-\overset{\vert}{\underset{\vert}{C}}-\ddot{\underset{\cdot\cdot}{O}}H$	$-\overset{\vert}{\underset{\vert}{C}}-\ddot{\underset{\cdot\cdot}{O}}-\overset{\vert}{\underset{\vert}{C}}-$
General formula	RH	$RCH=CH_2$ $RCH=CHR$ $R_2C=CHR$ $R_2C=CR_2$	$RC\equiv CH$ $RC\equiv CR$	ArH	RX	ROH	ROR
Specific example	CH_3CH_3	$CH_2=CH_2$	$HC\equiv CH$		CH_3CH_2Cl	CH_3CH_2OH	CH_3OCH_3
IUPAC name	Ethane	Ethene	Ethyne	Benzene	Chloroethane	Ethanol	Methoxymethane
Common name[a]	Ethane	Ethylene	Acetylene	Benzene	Ethyl chloride	Ethyl alcohol	Dimethyl ether

[a] These names are also accepted by the IUPAC.

♦ Summary (cont.)

Family						
Amine	**Aldehyde**	**Ketone**	**Carboxylic Acid**	**Ester**	**Amide**	**Nitrile**
						
RNH_2 R_2NH R_3N	$R\overset{\overset{O}{\|}}{C}H$	$R\overset{\overset{O}{\|}}{C}R'$	$R\overset{\overset{O}{\|}}{C}OH$	$R\overset{\overset{O}{\|}}{C}OR'$	$R\overset{\overset{O}{\|}}{C}NH_2$ $R\overset{\overset{O}{\|}}{C}NHR'$ $R\overset{\overset{O}{\|}}{C}NR'R''$	RCN
CH_3NH_2	$CH_3\overset{\overset{O}{\|}}{C}H$	$CH_3\overset{\overset{O}{\|}}{C}CH_3$	$CH_3\overset{\overset{O}{\|}}{C}OH$	$CH_3\overset{\overset{O}{\|}}{C}OCH_3$	$CH_3\overset{\overset{O}{\|}}{C}NH_2$	$CH_3C{\equiv}N$
Methanamine	Ethanal	Propanone	Ethanoic acid	Methyl ethanoate	Ethanamide	Ethanenitrile
Methylamine	Acetaldehyde	Acetone	Acetic acid	Methyl acetate	Acetamide	Acetonitrile

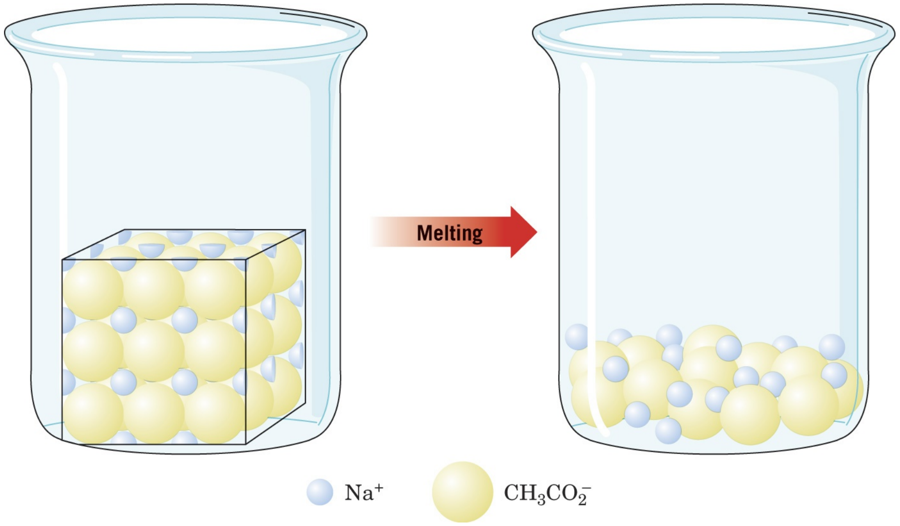
- **Physical Properties and Molecular Structure**
  - **The strength of intermolecular forces (forces between molecules) determines the physical properties (*i.e*. melting point, boiling point and solubility) of a compound**
  - **Stronger intermolecular forces result in high melting points and boiling 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**



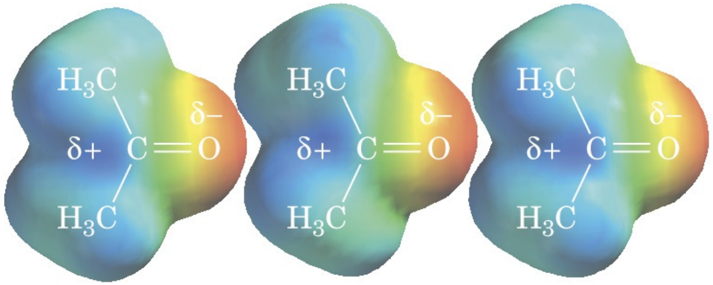
Compound	Structure	mp (°C)	bp (°C) (1 atm)[a]
Methane	CH_4	− 182.6	− 162
Ethane	CH_3CH_3	− 183	− 88.2
Ethene	$CH_2\text{"}CH_2$	− 169	− 102
Ethyne	$HC\#CH$	− 82	− 84 subl
Chloromethane	CH_3Cl	− 97	− 23.7
Chloroethane	CH_3CH_2Cl	− 138.7	13.1
Ethyl alcohol	CH_3CH_2OH	− 115	78.5
Acetaldehyde	CH_3CHO	− 121	20
Acetic acid	CH_3CO_2H	16.6	118
Sodium acetate	CH_3CO_2Na	324	dec
Ethylamine	$CH_3CH_2NH_2$	− 80	17
Diethyl ether	$(CH_3CH_2)_2O$	− 116	34.6
Ethyl acetate	$CH_3CO_2CH_2CH_3$	− 84	77

[a] In this table dec = decomposes and subl = sublimes.

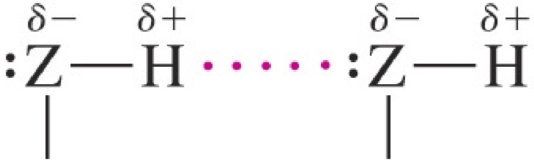
- **Ion-Ion Forces**
  - **Ion-ion forces are between positively and negatively charged ions**
  - **These are very strong forces that hold a solid compound consisting of ions together in a crystalline lattice**
    - **Melting points are high because a great deal of energy is required to break apart the crystalline lattice**
  - **Boiling points are so high that organic ions often decompose before they boil**
  - **Example: Sodium acetate**



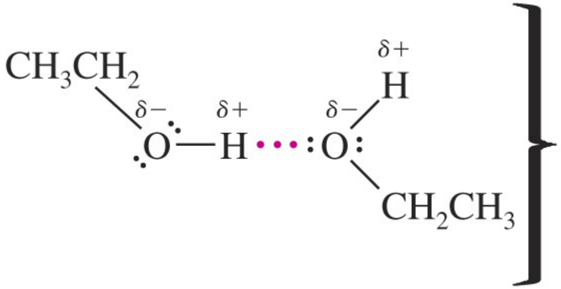
- **Dipole-Dipole Forces**
  - **Dipole-dipole forces are between molecules with permanent dipoles**
    - **There is an interaction between δ+ and δ- areas in each molecule; these are much weaker than ion-ion forces**
    - **Molecules align to maximize attraction of δ+ and δ- parts of molecules**
    - **Example: acetone**



- **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)**

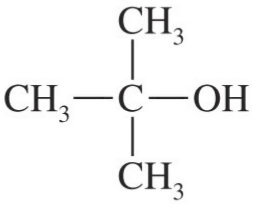


- **Example**
  - **Ethanol (CH_3CH_2OH) has a boiling point of +78.5°C; its isomer methyl ether (CH_3OCH_3) has a boiling point of -24.9°C**
    - **Ethanol molecules are held together by hydrogen bonds whereas methyl ether molecules are held together only by weaker dipole-dipole interactions**



The dotted bond is a hydrogen bond. Strong hydrogen bonding is limited to molecules having a hydrogen atom attached to an O, N, or F atom.

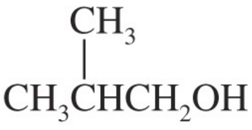
  - **A factor in melting points is that symmetrical molecules tend to pack better in the crystalline lattice and have higher melting points**



***tert*-Butyl alcohol**
(mp 25°C)

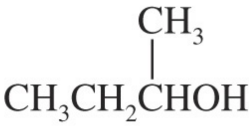
$CH_3CH_2CH_2CH_2OH$

Butyl alcohol
(mp −90°C)



$CH_3\overset{CH_3}{\overset{|}{C}}HCH_2OH$

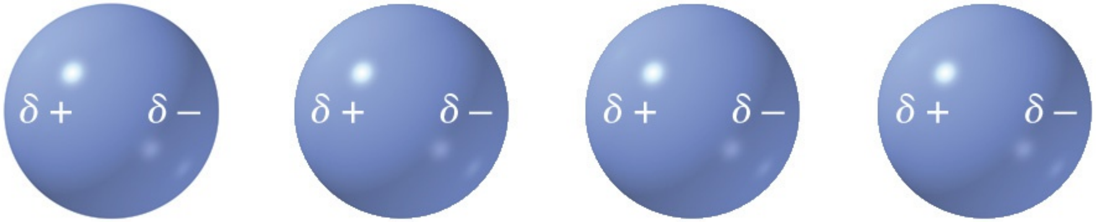
Isobutyl alcohol
(mp −108°C)



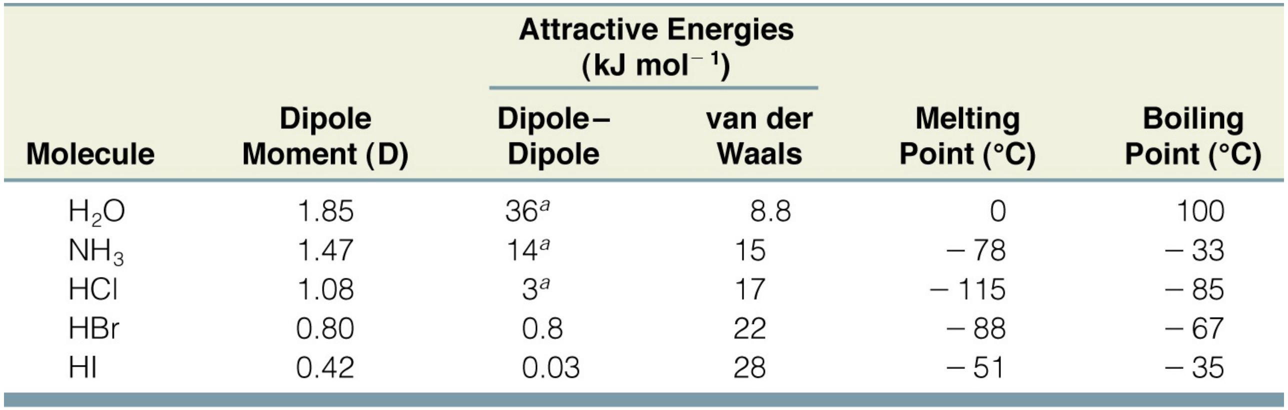
$CH_3CH_2\overset{CH_3}{\overset{|}{C}}HOH$

***sec*-Butyl alcohol**
(mp −114°C)

- 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



- **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)**

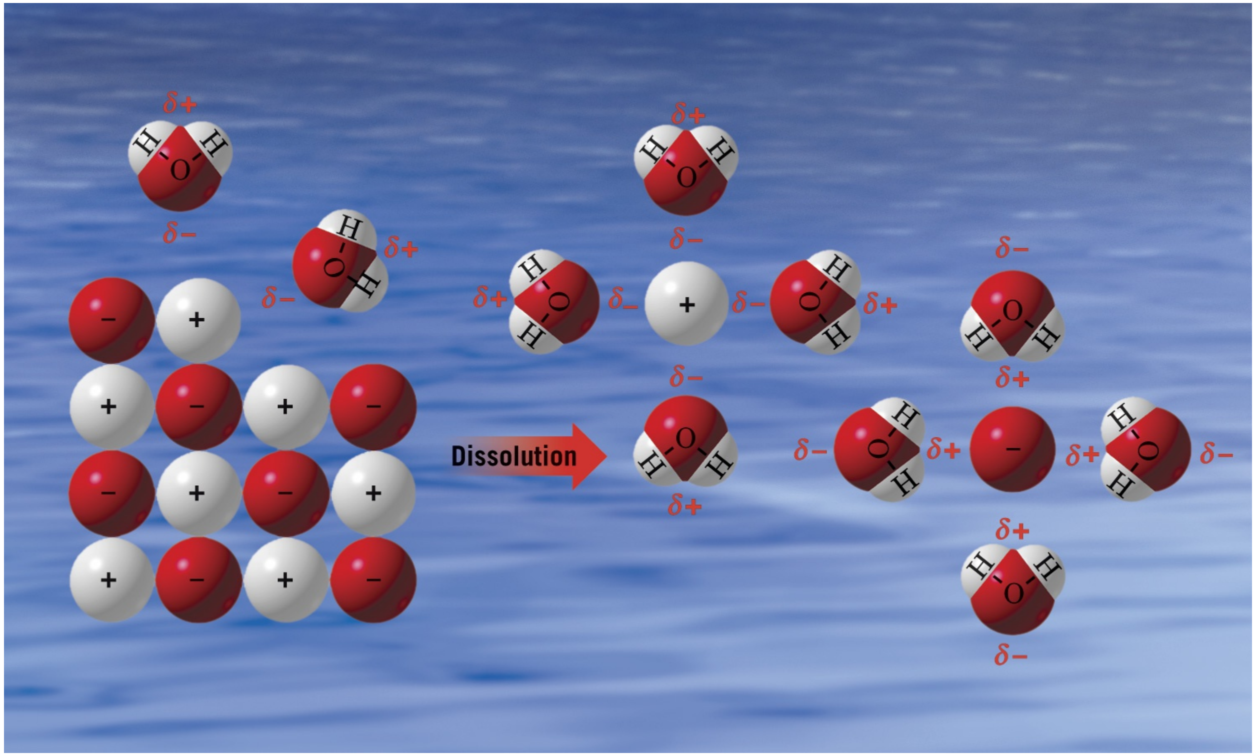


Molecule	Dipole Moment (D)	Attractive Energies ($kJ\ mol^{-1}$) Dipole–Dipole	van der Waals	Melting Point (°C)	Boiling Point (°C)
H_2O	1.85	36[a]	8.8	0	100
NH_3	1.47	14[a]	15	− 78	− 33
HCl	1.08	3[a]	17	− 115	− 85
HBr	0.80	0.8	22	− 88	− 67
HI	0.42	0.03	28	− 51	− 35

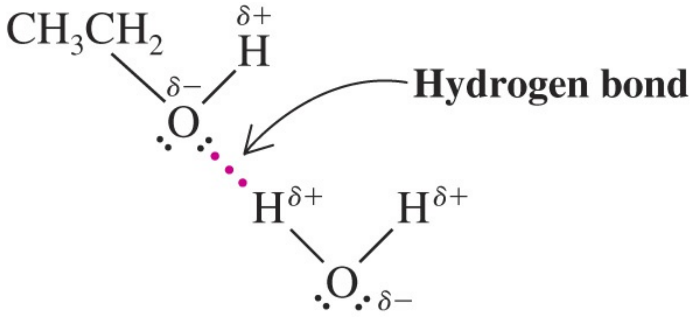
[a] These dipole–dipole attractions are called hydrogen bonds.

- **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 (CH_4) has a boiling point of -162°C whereas ethane (C_2H_6) has a boiling point of -88.2°C**

- **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**



- **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**

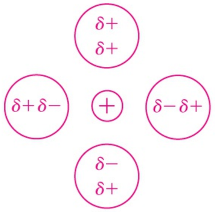
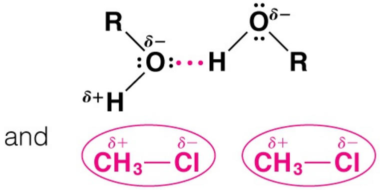


- **A large alkyl group can overwhelm the ability of the polar group to solubilize a molecule in water**
  - **Decyl alcohol is only slightly soluble in water**
  - **The large alkyl portion is hydrophobic ("water hating") and overwhelms the capacity of the hydrophilic ("water loving") hydroxyl**


$$\overbrace{CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2}^{\text{Hydrophobic portion}}OH$$

- **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	⊕ ⊖	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})	$-\overset{\delta-}{Z}:\cdots\overset{\delta+}{H}-$	
van der Waals	Variable	Transient dipole	Interactions between methane molecules

- **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**

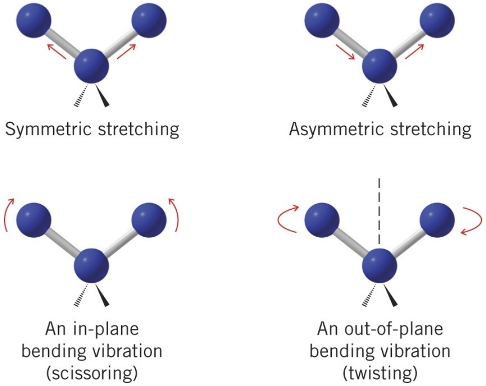
- **Infrared Spectrometer**
  - **An infrared spectrometer detects the frequencies absorbed by the sample molecule**
  - **Light of all the various IR frequencies is transmitted to the molecule and the frequencies absorbed are recorded**
  - **The absorption frequencies are specified as wavenumbers in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

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

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

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

A stretching vibration



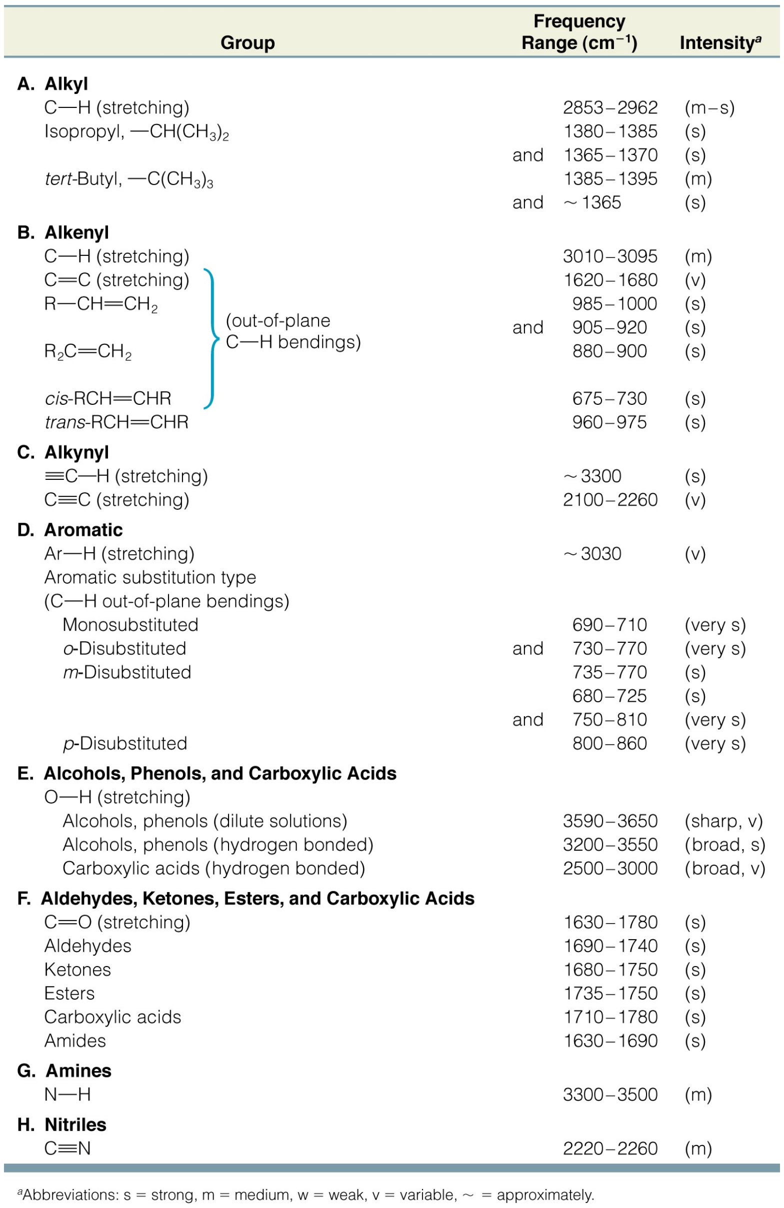
- **The actual relative frequency of vibration can be predicted**
  - **Bonds with lighter atoms vibrate faster than those with heavier atoms**

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

- **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})
$C\equiv C$	2100–2260
$C\equiv N$	2220–2260
$C=C$	1620–1680
$C=O$	1630–1780

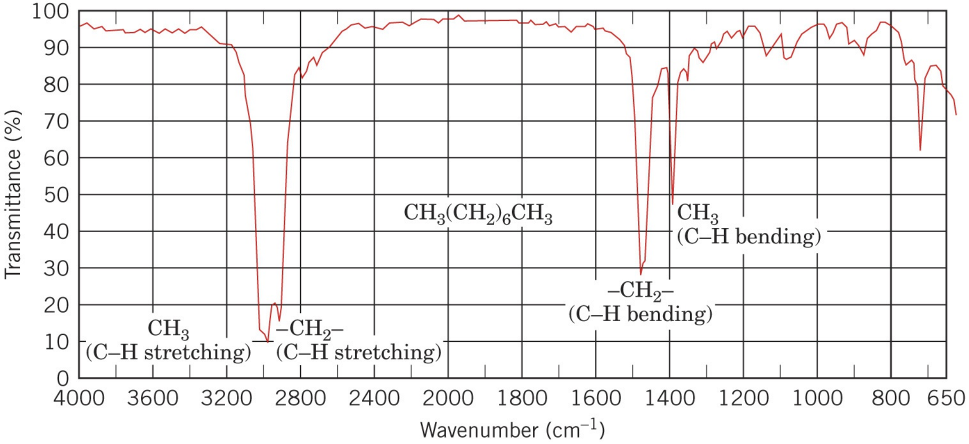
- **The IR spectrum of a molecule usually contains many peaks**
  - **These peaks are due to the various types of vibrations available to each of the different bonds**
  - **Additional peaks result from overtone (harmonic) peaks which are weaker and of lower frequency**
  - **The IR is a “fingerprint”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



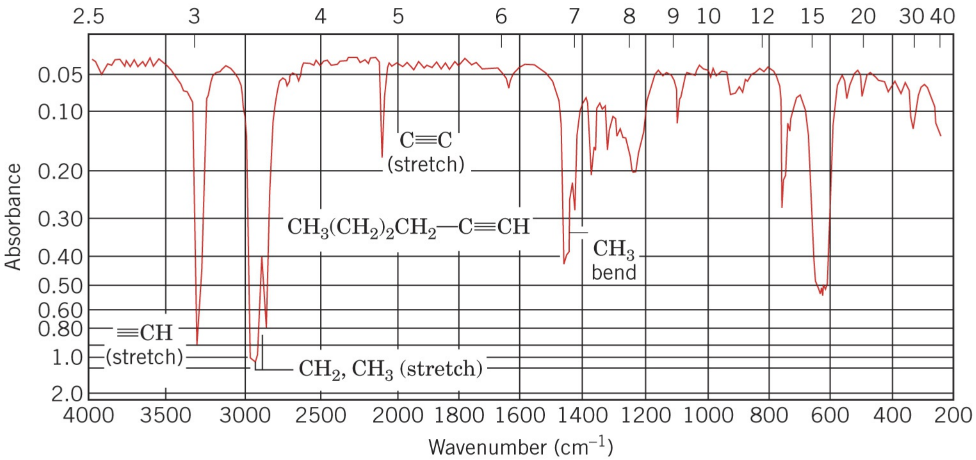
- **Interpreting IR Spectra**
  - **Generally only certain peaks are interpreted in the IR**
    - **Those peaks that are large and above 1400 cm^{-1} are most valuable**

- **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 sp^2 centers appear at about 3080 cm^{-1}**
    - **C-H bonds at sp^3 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**

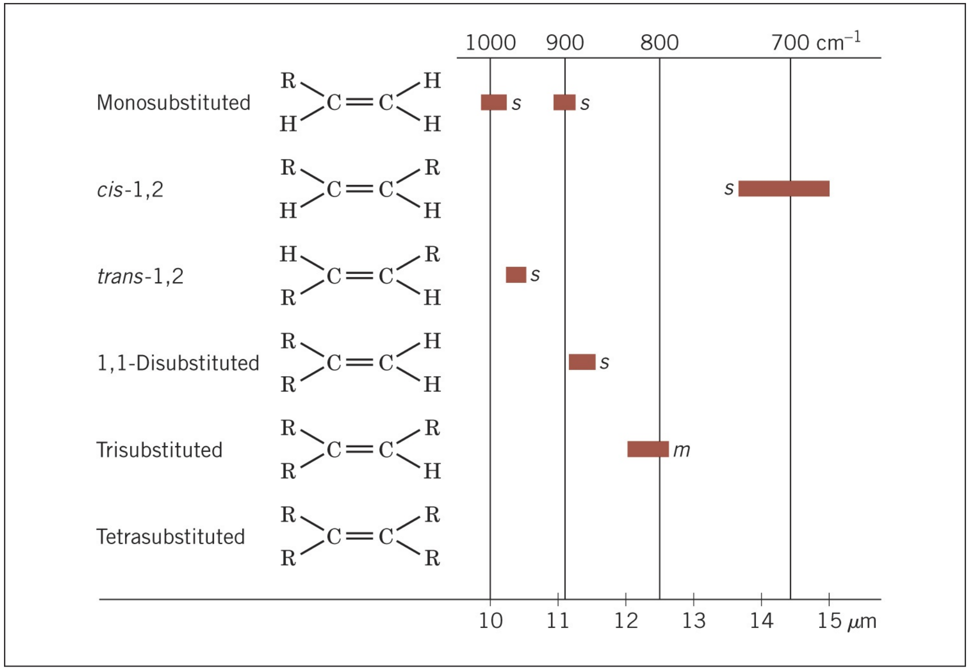
- **Example: octane**



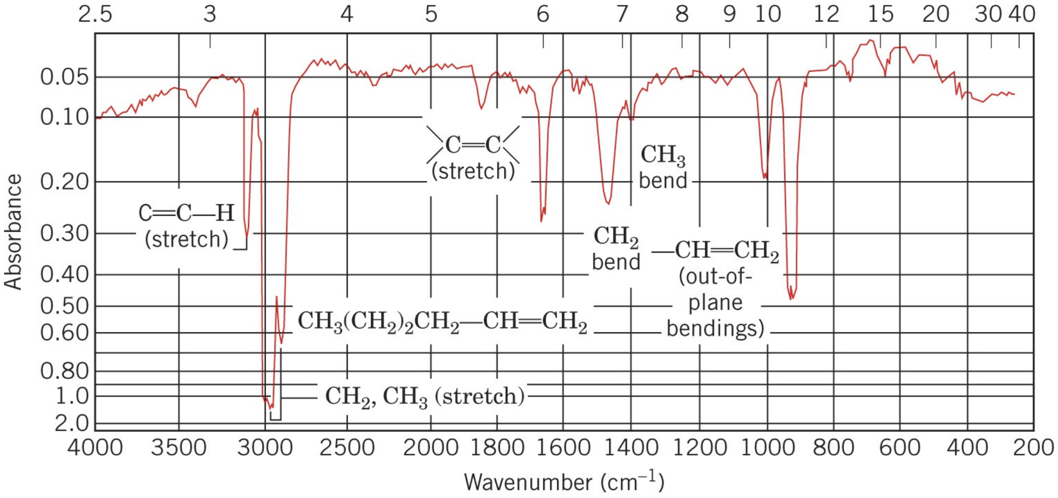
- **Example: 1- hexyne**



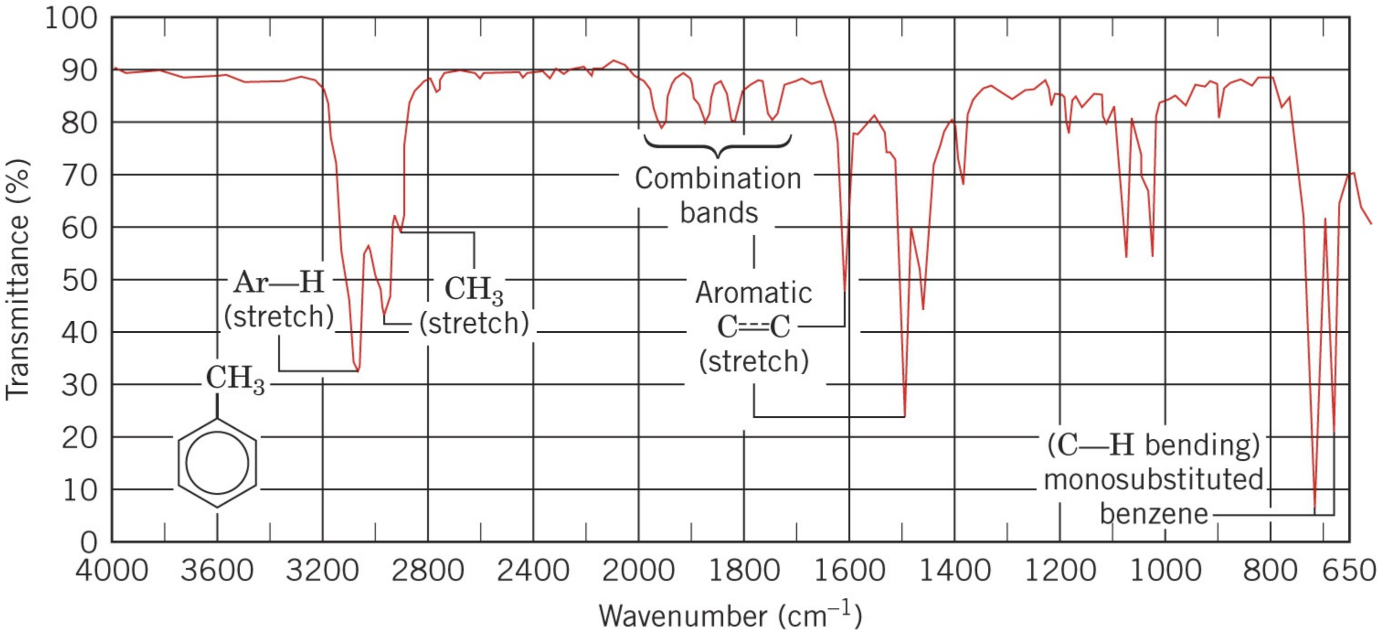
- **Alkenes**
  - **The C-H bending vibration peaks located at 600-1000 cm^{-1} can be used to determine the substitution pattern of the double bond**



- **Example: 1-hexene**

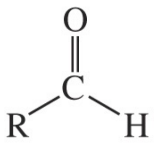


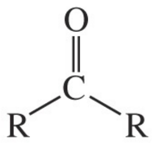
- **Aromatic Compounds**
  - **The C-C bond stretching gives a set of characteristic sharp peaks between 1450-1600 cm^{-1}**
  - **Example: Methyl benzene**

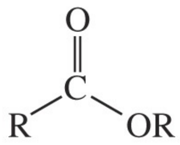


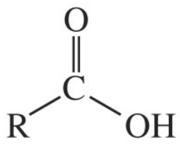
Other Functional Groups

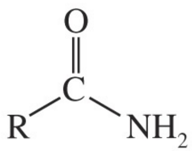
- **Carbonyl Functional Groups**
  - **Generally the carbonyl group gives a strong peak which occurs at 1630-1780 cm^{-1}**
    - **The exact location depends on the actual functional group present**


Aldehyde
1690–1740 cm^{-1}

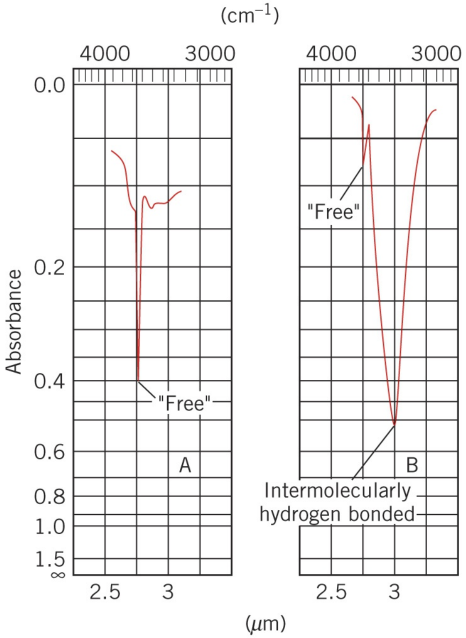

Ketone
1680–1750 cm^{-1}


Ester
1735–1750 cm^{-1}


Carboxylic acid
1710–1780 cm^{-1}


Amide
1630–1690 cm^{-1}

- **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 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 cm^{-1}**
    - **A phenol has a hydroxyl group directly bonded to an aromatic ring**

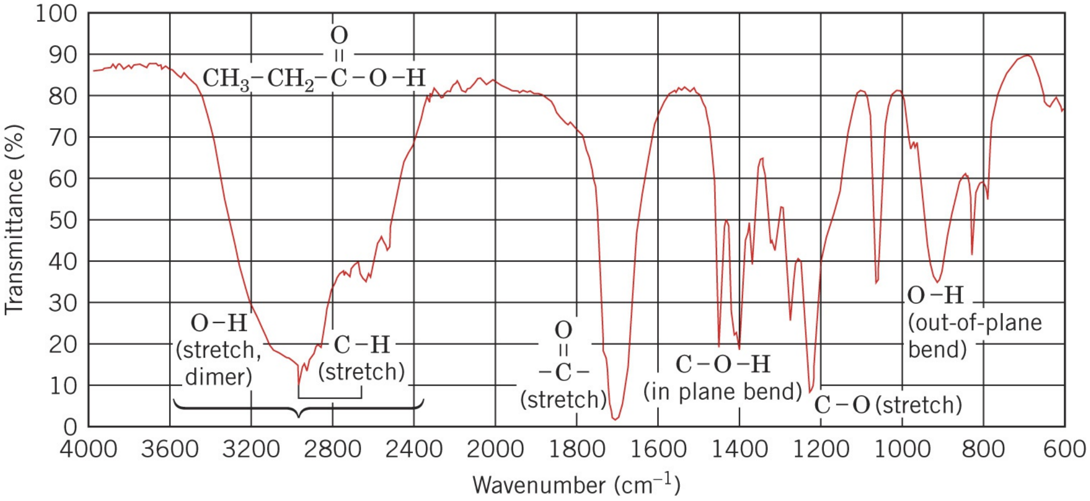


(*a*) (*b*)

Carboxylic Acids

  - The carbonyl peak at 1710-1780 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**



- **Amines**
  - **Very dilute solution of 1^o and 2^o amines give sharp peaks at 3300-3500 cm^{-1} for the N-H stretching**
    - **1^o amines give two peaks and 2^o amines give one peak**
    - **3^o 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**