Organic Chemistry Background

- **In excess of 10,000,000 compounds of C**
- **Fewer than 500,000 compounds of elements other than C**
- **Almost all C compounds are found in living things. Exceptions are CO, CO_2, CO_3^{-2}, CN^{-1}, C^{-4}**
- **Why does C form so many compounds?**
  Catenation - the ability to form long chains and rings. This ability stems from the s^2p^2 electron configuration and its ability to rearrange (hybridize) these electrons in order to facilitate bonding. The theory of bonding which takes into account hybridization and the overlap of electron clouds to form sigma (s) and pi (p) bonds is called the <u>valence bond theory</u>.

What are the types of rearrangements?

- **4 equal energy orbitals which will form 4 equal single bonds. This gives a tetrahedral geometry. The name of the hybridization is sp^3 and the carbon is said to be saturated.**
- **3 equal energy orbitals and one unequal which will form 2 single bonds and 1 double bond. This gives a trigonal planar geometry. The name of the hybridization is sp^2 and the carbon is unsaturated.**
- **2 equal energy orbitals and 2 unequal orbitals which will form 1 single bond and 1 triple bond or 2 double bonds. The geometry is linear. The name of the hybridization is sp and the carbon is unsaturated.**

The Alkanes

Alkanes are saturated hydrocarbons with chains (linear or branched). There major source is crude oil. They are nonpolar molecules held together by dispersion forces.

CH_4	methane
C_2H_6	ethane
C_3H_8	propane
C_4H_{10}	butane
C_5H_{12}	pentane
C_6H_{14}	hexane
C_7H_{16}	heptane
C_8H_{18}	octane
C_9H_{20}	nonane
$C_{10}H_{22}$	decane

There are so many isomers that exist in organic chemistry that we almost always write the formulas as structural formulas or condensed structural formulas. For example C_4H_{10} can exist in two different forms and we must therefore have two different names. The naming system that is used is called the IUPAC system. For simple alkanes and related compounds:

- **Look for the longest carbon chain - this is called the parent chain and determines the root word for the name**
- **Look for the substituent (radical) attached to the parent chain. This substituent will end in -yl.**
- **Put the position number in front of the radical and attach to the root word. Position numbers should be the lowest possible.**
- **If more than 1 radical is present, put in alphabetical order. If more than 1 of the same type use a prefix to indicate the number.**

Cycloalkanes

Saturated hydrocarbons with rings

A. Naming

- **Count the number of C atoms in the ring and use the prefix cyclo**
- **When radical are present, number the carbons such that the radicals have the lowest position numbers possible.**
- **Can use geometrical figure for a short-hand notation of the ring.**

Alkenes

Unsaturated hydrocarbons that have one or more C=C groups and exist in chains

A. Naming

- **Change the -ane ending to -ene**
- **The parent chain must contain the double bond**
- **The position of the double bond must be specified if the chain is longer than 3 C. This is accomplished by adding a prefix to the beginning. (Example   2-butene)**
- **The parent chain is numbered so that the double bond gets lowest position number. This takes priority over the attachment of radicals.**
- **If more than 1 double bond is present, use the prefix di, tri, tetra, etc. with the -ene ending.**

B. C=C bonds are much more reactive than C-C bonds and are very useful to make other compounds.

Cycloalkenes

A. Naming

- Use the rules for cycloalkanes plus . . .
- Number the ring starting at the C=C bond. The direction (clockwise or counterclockwise) is determined by the position of the radicals. Number such that they get the lowest position number.

Alkynes

Unsaturated hydrocarbons that have 1 or more C^{o}C bonds and exist in chains.

A. Naming

- Change the -ane ending to -yne
- If a C=C and C^{o}C occur the parent chain is numbered for the C=C

B. C^{o}C is very reactive

Aromatics

unsaturated hydrocarbons with delocalized bonding in a 6-membered ring

A. All based on the compound benzene (C_6H_6)

- **Bond lengths all the same**
- **Molecule more stable than expected**
- **Each C hybridized sp^2. The 6 p orbitals in the ring share their p electrons. This delocalizes the electrons.**

B. Naming

- **If one ring is present the rules are similar to the cycloalkanes but many common names are used.**
- **Disubstituted benzenes can be named without position numbers by using the prefixes ortho (1,2), meta (1,3), and para (1,4).**
- **Radical of benzene is named phenyl.**

Fossil Fuels

Fossil fuels are hydrocarbon deposits formed from the remains of once living organisms

A. History of use

Early 1800's - wood dominant source

Late 1800's - switch to coal

Early 1900's - oil and natural gas dominant

B. Today (approximate)

Oil	**40 to 45 %**
Coal	**20 to 25%**
Natural gas	**20-25%**
Hydroelectric	**5%**
Nuclear	**5%**

C. **Our energy problems in the US revolve around the problem than we import much of our oil, which is the predominant energy source in the transportation sector of the economy. The US reserves of oil (at present consumption) are less than 50 years, with natural gas being somewhat greater (50 to 100), and uranium also being less than 100 years. Coal reserves are <u>much higher</u>, but coal is a naturally dirty fuel (Sulfur contamination) when burned as a solid.**

D. **Petroleum (Oil) - a complex mixture of hydrocarbons found underground, trapped under pressure**

- **Refining - the separation of petroleum into useful components by fractional distillation**

- **Chemical alterations -**
  1. **cracking - long molecules can be broken to short ones**
  2. **polymerization - short molecules can be made into longer one**
  3. **reforming - alkanes can be converted into aromatics**
  4. **isomerization - straight chains can be changed to branched chains**
- **Removal of sulfur compounds**

D. Gasoline

- **As the piston in an internal combustion engine moves up it compresses the gas/air mixture. If it ignites too soon on its upward travel, power is lost and we say the engine "knocks". The octane rating is a measure of the ability to reduce this knocking. Branched chain hydrocarbons and aromatics ignite more slowly and have a higher octane number. Straight chain molecules ignite faster and have a lower octane number.**

  heptane - octane # 0

  2,2,4-trimethyl pentane - octane # 100

- **Straight run gasoline from the distillation of crude oil has an octane of 50-55. Octane number is increased by the use of isomerization, reforming and the addition of antiknock agents such as tetraethyl Pb (now banned), ethanol, or methyl t-butyl ether.**

Energy and Power Units

Energy/heat/work	Power
British Thermal Units (BTU)	Horsepower (hp)
Joules (J)	watts and kilowatts (w and kw)
calories and Calories (kcal)	
kilowatt hours (kwh)	
Quad (10^{15} BTU)	

Energy is the property of matter that allows work to be done and heat to be generated.

Power is the rate at which energy is produced, transferred or used. (energy/time)

Energy Alternatives

- **Energy is a global problem, an economic problem, a political problem, and a scientific problem.**
- **The U.S. has about 5% of the world's population but uses 20% of the world's energy. The U.S. uses about 90 quads of energy a year.**
- **We continue to mainly use nonrenewable fossil fuels.**
- **Although we are not running out of energy itself, we are running out of concentrated sources of energy. This is important because it gets more difficult to extract energy from diffuse sources.**
- **It is a basic law of thermodynamics that we cannot take all the energy from one place and convert it to useful work. Some is always lost.**

Possible solutions

- **Use less energy (conserve).**
- **Change to alternative sources other than oil, natural gas or coal.**

  Nuclear (energy very concentrated and can be released by fission and fusion) - problems with fission waste, technology problems with fusion

  Solar - (useful for heating and the production of electricity) very spread out, not available all the time

  Biomass - (uses the power of photosynthesis) - biofuels may produce air pollutants

  Tidal - limited use

  Geothermal - limited use

- **Change coal and other resources (like trash) into other more easily used energy sources.**

Alcohols (R-OH)

A. **Naming**
   - **Replace parent ending "e" with an "ol"**
   - **If necessary specify the position number**
   - **If multiple -OH groups are present use Greek prefixes di-, tri-, etc.**

B. **Small alcohols are water soluble**

C. **Many common names are used**

IUPAC	Common
methanol	methyl alcohol, wood alcohol
ethanol	ethyl alcohol, grain alcohol
1,2-ethanediol	ethylene glycol
2-propanol	isopropyl alcohol, rubbing alcohol
1,2,3-propanetriol	glycerol, glycerin
phenol	

Ethers (R-O-R')

A. Naming

Common names - name radicals and end in the word ether

IUPAC - choose the longest carbon chain as the parent, the -O-R group that is left is the radical. These radicals are "oxy" radicals.

$-O-CH_3$	methoxy
$-O-CH_2-CH_3$	ethoxy

B. Properties

Weak intermolecular forces, high VP

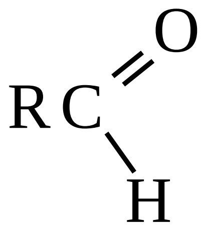
Very flammable

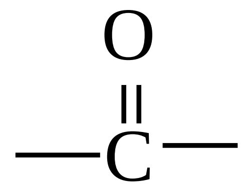
Excellent solvent

Small ethers used as anesthetics in medicine

A Gasoline additive is MTBE

Aldehydes



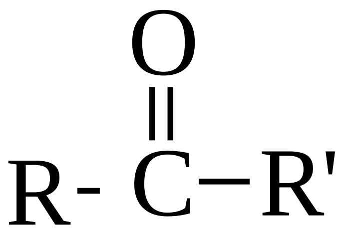
A. Contains the carbonyl group 

B. Naming

Change "-e" of alkane to "-al"

IUPAC	Common
methanal	formaldehyde
ethanal	acetaldehyde
benzaldehyde	"almond flavor"
4-hydroxy-3-methoxybenzaldehyde	"vanillin"

Ketones



A. **Contains a carbonyl**

B. **Naming (IUPAC)**

Locate the longest carbon chain with a carbonyl

Replace “-e” with “-one”

Indicate position number

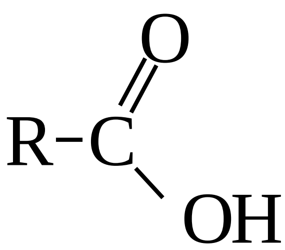
Use Greek prefixes if more than one carbonyl present

C. **Naming (Common)**

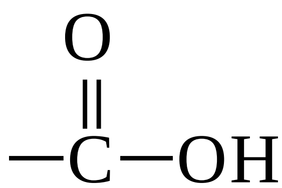
Name the R radicals and end with ketone

IUPAC	**Common**
2-propanone	**dimethyl ketone, acetone**

Carboxylic Acids



A. Contains the carboxyl group



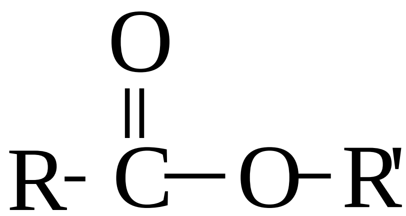
B. Naming

Locate the longest carbon chain with the carboxyl group

Replace “-e” with “-oic acid”

IUPAC	**Common**
methanoic acid	**formic acid**
ethanoic acid	**acetic acid**
ethanedioic acid	**oxalic acid**
benzoic acid	

Esters



A. Naming

The carboxylate part of the ester is named from the acid it is derived from. The R’ radical is named as usual.

B. Properties

Many used as flavorings

Used in medicine (aspirin)

Amines

A. **Can be considered to be derivatives of NH_3 where the H is replaced by R groups**

B. **Naming**

List R groups in alphabetical order and end in the word amine [Easier for amines with 1 N]

or

Name the $-NH_2$ group as the amino group [Easier for amines with more than 1 N]

C. Properties

fishy and foul smells

adrenal gland secretions

D. Examples

ethylmethylpropylamine

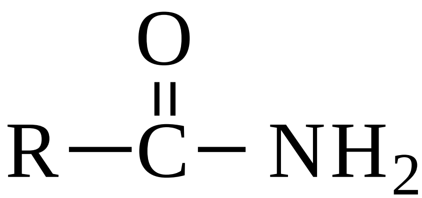
1,4-diaminobutane , “putrescine”

1,5-diamopentane, “cadaverine”

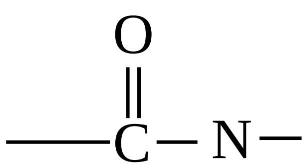
“epinephrine” or “adrenaline”

Caffeine, nicotine, morphine are all amines called alkaloids and are derived from plants

Amides



All amides contain the amide linkage, also called the peptide linkage.



A. Naming simple amides

Think of a simple amide as a carboxylic acid with $-NH_2$ replacing the -OH.

For naming, replace the -ic or -oic ending of the acid with -amide.

Example - methanamide “formamide”, ethanamide “acetamide”, benzamide

B. Properties and uses

The amide linkage holds proteins together and is the basis for polymers like nylon.

Pain relievers like acetaminophen contain the amide linkage.

Polymers

About 80% of the organic chemical industry is devoted to making polymers.

A. Background

- **Polymers are macromolecues which have molecular weights ranging from the thousands to the millions.**
- **Polymers are made from low molecular weight molecules linked together. The repeating unit is called a <u>monomer</u>. The chains can be physically entangled and chemically cross-linked (bonded) together.**
- **Important <u>properties</u> of polymers are their *memory* (elasticity), their *high viscosity*, and their *poor solubility in water*.**
- **Important <u>applications</u> of polymers are in *fibers*, *elastomers*, and *plastics***
- **Two important types of polymers are *addition* and *condensation* polymers.**

B. Addition Polymers

- **The polymer is produced from the simple addition of monomers to give the polymer, with no other products formed.**
- **<u>The monomers are low molecular weight alkene derivatives, derived from petroleum.</u>**
- **The process of linking the molecules together proceeds by the initial formation of free radicals by heating or other starter reactions. The free radicals attack other monomers and link the monomers together.**
- **Polyethylene, polypropylene, polyvinyl chloride (PVC), and teflon are good examples.**

C. Condensation polymers

- **Polymers formed from the reaction of 2 unlike molecules to give a large molecule. An additional small molecule such as water is also made in the process.**
- **<u>The monomers must be bifunctional</u>.**
- **Polyester (diacid + dialcohol) and nylon (diacid + diamine) are good examples.**