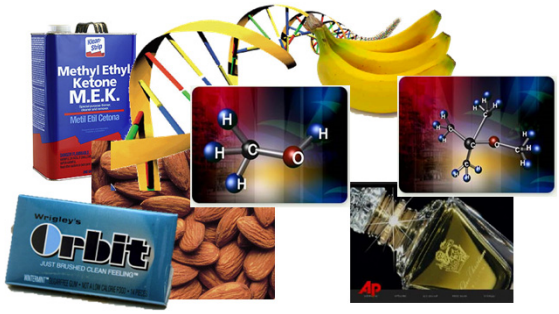
Organic Chemistry: The Chemistry of Carbon Compounds

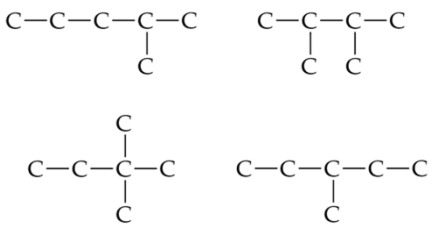


Diversity of Carbon

- Creates four bonds
- Can create multiple bonds (double, triple)
- Valence electrons close to nucleus
- Ability to "string together" into long chains
- High stability (high bond energies)
- Variety of geometries possible

Isomers

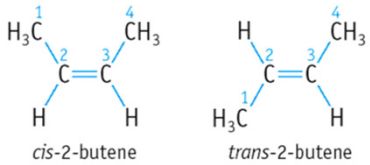
Structural: Same formula, different structure



Isomers

Stereoisomers: Same formula with similar attachments but different orientations.

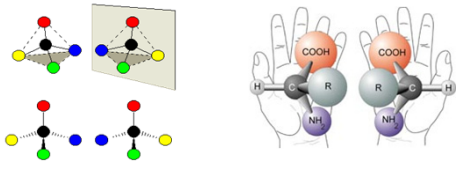
Geometric isomers:



Note that carbons are not free to rotate around double bond.

Isomers

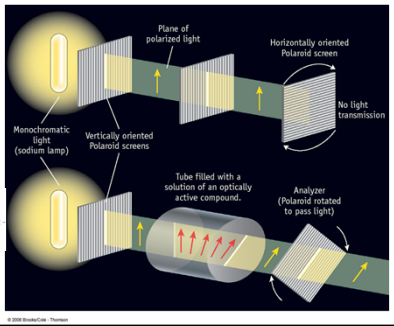
Optical isomers: Nonsuperimposable mirror image
(termed **chiral**; Pairs of chiral molecules are called **enantiomers**)



Molecules cannot be rotated to be the same

Chiral molecules can rotate plane polarized light (levorotary (levorotatory), dextrorotary (dextrorotatory)

Examples:
Lactic Acid,
alanine
(amino acid)
and simple
sugars
glucose
(dextrose)
and fructose
(levulose)

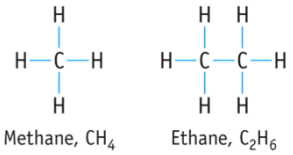


Hydrocarbons - Alkanes

Hydrocarbons: Containing only carbon and hydrogen

Alkanes: Consisting of only single-bonded atoms (saturated)

General Formula (C_nH_{2n+2})



Methane, CH_4 Ethane, C_2H_6

Alkane Nomenclature

The name of an alkane is dependant upon the number of carbons in the chain using the following prefixes:

# carbons	Prefix
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	non
10	dec

Melting and boiling point increase with increased chain length

The suffix "ane" is added to designate the molecule as an alkane.

Often times you will find shorter branches of carbons off of the longest (main or parent) chain. These branches are known as alkyl groups, branches or substituents.

They are named using the same prefixes as before but using -yl as a suffix on the name.

Naming Branched Chain Alkanes

1. Find the longest continuous chain of hydrocarbon (remember that they may bend around corners). This is your parent chain.

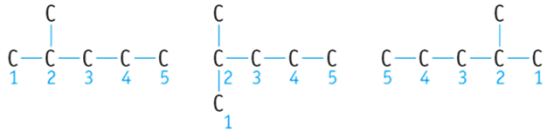
2. Number the parent chain beginning from the end closest to the first branch.

3. Identify the alkyl groups and the carbon number on the parent chain they are attached to.

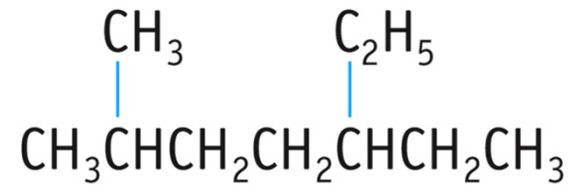
4. List the alkyl groups in alphabetical order and the number where the attachment occurs. (Separate numbers from words with hyphens).

5. Finally, list the parent name.

Beware of carbon chains that look different, but are the same. All three of these below are 2-methylpentane. These are NOT isomers.



Name this compound



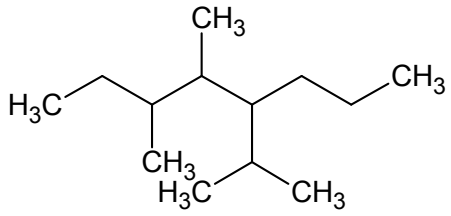
5-ethyl-2-methylheptane

Condensed structural formula	Name
$-CH_3$	methyl
$-CH_2CH_3$	ethyl
$-CH_2CH_2CH_3$	propyl
$-CH_2CH_2CH_2CH_3$	butyl
$-CHCH_3$ $\quad\quad\vert$ $\quad\quad CH_3$	isopropyl
$-CH_2CHCH_3$ $\quad\quad\quad\vert$ $\quad\quad\quad CH_3$	isobutyl
$-CHCH_2CH_3$ $\quad\quad\vert$ $\quad\quad CH_3$	sec-butyl
$\quad\quad CH_3$ $\quad\quad\vert$ $-CCH_3$ $\quad\quad\vert$ $\quad\quad CH_3$	tert-butyl

tert and sec are not used in alphabetizing but iso is because it is part of the name.

Prefixes like di, tri and tetra are not used in alphabetizing.

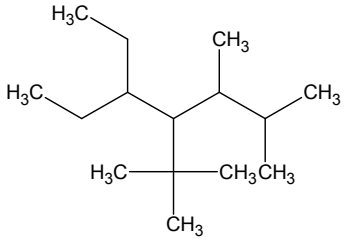
Example: Name the following:



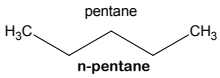
5-isopropyl-3,4-dimethyloctane

Example: Draw the structure for:

4-*tert*-butyl-5-ethyl-2,3-dimethylheptane

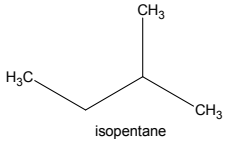


Example: Draw and name all the structural isomers of pentane.



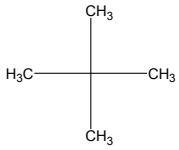
pentane

n-pentane



isopentane

2-methylbutane



neopentane

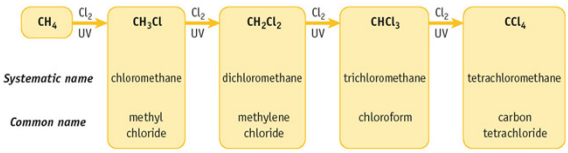
2,2-dimethylpropane

Properties of Alkanes

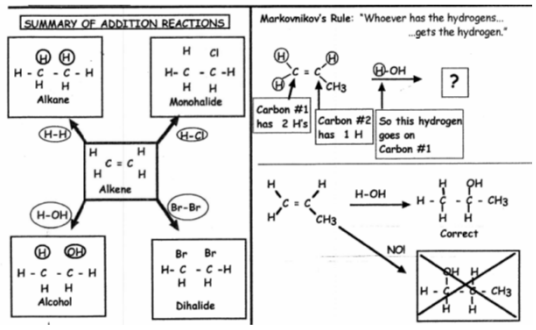
Alkanes burn in oxygen to produce carbon dioxide and water (combustion)

$CH_{4(g)} + 2O_{2(g)} \rightarrow CO_{2(g)} + 2H_2O_{(l)}$ $\Delta H^o_{rxn} = -890.3kJ$

Alkanes undergo substitution reactions with chlorine gas (and other halogens)



In order for an alkane to be chiral, a compound must have at least one C atom attached to four different groups



Cycloalkanes

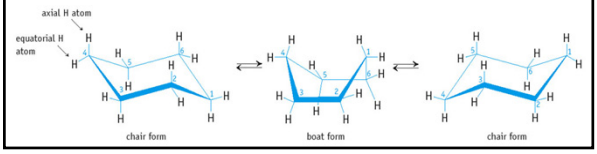
Single-bonded carbons can create rings (cycloalkanes) of the general formula, C_nH_{2n}

Cycloalkanes are named the same way as alkanes, except the word "cyclo" is placed in front (e.g. pentane becomes cyclopentane)

Cyclopropane, C_3H_6

Cyclopropane and cyclobutane have "strained" bond angles that are much less than 109.5°

Cyclohexane can exist in either a "boat" or "chair" conformation.



Alkenes and Alkynes

Alkenes have one or more double bonded carbon atoms and have the general formula C_nH_{2n} (for a single double bond)

Alkynes have one or more triple bonded carbon atoms and have the general formula C_nH_{2n-2} (for a single triple bond)

Only alkenes exhibit cis/trans isomerism

The suffix ending on alkenes is "ene"
The suffix ending on alkynes is "yne"

Alkenes and Alkynes

The position(s) of the multiple bond(s) must be identified in the name.

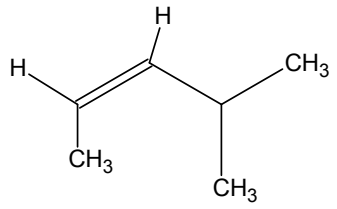
The parent chain is the longest chain containing the multiple bond(s).

Numbering begins from the end closest to the first multiple bond.

If more than one multiple bond appears, the prefixes di, tri, tetra, etc. must be used (e.g. octa-2,4-diyne)

Sample Questions

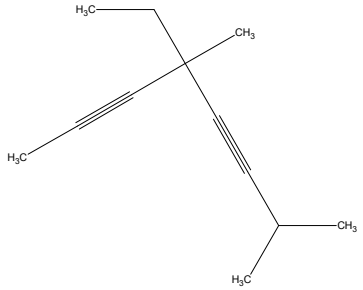
Name the following molecule:



4-methylpenta-cis-2-ene (4-methyl-cis-2-pentene)

Sample Questions

Name the following molecule:

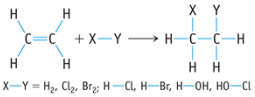


4-ethyl-4,7-dimethylocta-2,5-diyne

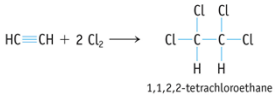
Properties of Alkenes and Alkynes

Alkenes and alkynes are *unsaturated* compounds (have fewer than the maximum number of hydrogens possible)

Addition Reactions:



When the addition involves H_2 to a double bond it is known as *hydrogenation*.

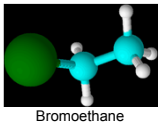


1,1,2,2-tetrachloroethane

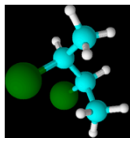
Examples:

1. Draw the structure of the compound obtained from the reaction of HBr with ethylene and name the compound.

2. Draw the structure of the product of the reaction of Br_2 with cis-but-2-ene (cis-2-butene) and name this compound.



Bromoethane



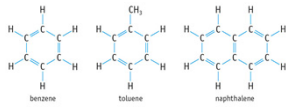
2,3-dibromobutane

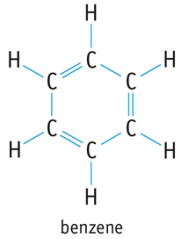
Aromatic compounds

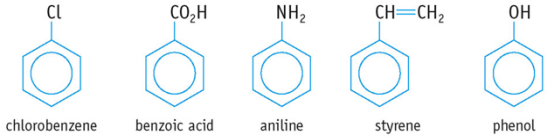
Compounds that contain the benzene ring are known as aromatic vs. those that don't which are called aliphatic

Discovered by Michael Faraday in 1825 (structure determined by August Kekulé)

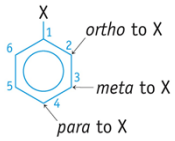
Benzene is a hybrid resonance structure

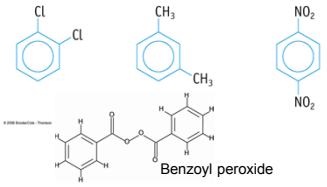






The terms ortho (o), meta (m) and para (p) are often used to identify substituent groups on benzene rings





Properties of Aromatic Compounds

Unusual stability associated with π bonding (resonance stabilization)

Substitution reactions are common among aromatic compounds

Nitration: $C_6H_{6(l)} + HNO_{3(l)} \xrightarrow{H_2SO_4} C_6H_5NO_{2(l)} + H_2O_{(l)}$

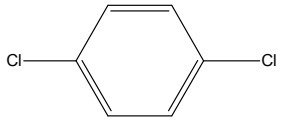
Alkylation: $C_6H_{6(l)} + CH_3Cl_{(l)} \xrightarrow{AlCl_3} C_6H_5CH_{3(l)} + HCl_{(g)}$

Halogenation: $C_6H_{6(l)} + Br_{2(l)} \xrightarrow{FeBr_3} C_6H_5Br_{(l)} + HBr_{(g)}$

Examples

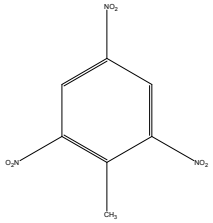
1. Draw the structure for 2,4,6-trinitrotoluene (TNT), where a nitro group is $-NO_2$ and toluene consists of a benzene ring with a methyl group attached.

2. Determine the two possible names for the following molecule.



Answers:

1.



2. Either p-dichlorobenzene or 1,4-dichlorobenzene

Chemical used to make mothballs and toilet bowl deodorizer tablets. Less toxic than naphthalene, but PDCB causes cancer in laboratory animals.

Functional Groups

Table 11.6 Common Functional Groups and Derivatives of Alkanes

Functional Group*	General Formula*	Class of Compound	Examples
F, Cl, Br, I	RF, RCl, RBr, RI	haloalkane	CH_3CH_2Cl, chloroethane
OH	ROH	alcohol	CH_3CH_2OH, ethanol
OR′	ROR′	ether	$(CH_3CH_2)_2O$, diethyl ether
NH_2†	RNH_2	(primary) amine	$CH_3CH_2NH_2$, ethylamine
O ‖ —CH	RCHO	aldehyde	CH_3CHO, ethanal (acetaldehyde)
O ‖ —C—R′	RCOR′	ketone	CH_3COCH_3, propanone (acetone)
O ‖ —C—OH	RCO_2H	carboxylic acid	CH_3CO_2H, ethanoic acid (acetic acid)
O ‖ —C—OR′	RCO_2R'	ester	$CH_3CO_2CH_3$, methyl acetate
O ‖ —C—NH_2	$RCONH_2$	amide	CH_3CONH_2, acetamide

Alcohols

Have hydroxyl groups –OH

Names end with "ol"

Hydroxyl group identified by the carbon in the parent it is attached to

Ethanol can be produced by the addition of water to ethylene

Has hydrogen bonding intermolecular attractions

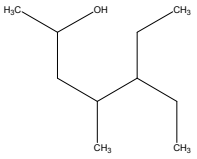
R-OH

Alcohol

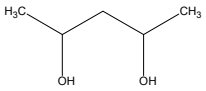
Table 11.7 Some Important Alcohols

Condensed Formula	BP (°C)	Systematic Name	Common Name	Use
CH_3OH	65.0	methanol	methyl alcohol	fuel, gasoline additive, making formaldehyde
CH_3CH_2OH	78.5	ethanol	ethyl alcohol	beverages, gasoline additive, solvent
$CH_3CH_2CH_2OH$	97.4	1-propanol	propyl alcohol	industrial solvent
$CH_3CH(OH)CH_3$	82.4	2-propanol	isopropyl alcohol	rubbing alcohol
$HOCH_2CH_2OH$	198	1,2-ethanediol	ethylene glycol	antifreeze
$HOCH_2CH(OH)CH_2OH$	290	1,2,3-propanetriol	glycerol (glycerin)	moisturizer in consumer products

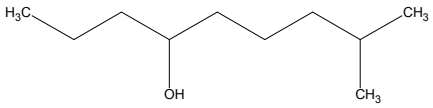
Examples: Name the following compounds



5-ethyl-4-methylheptan-2-ol



pentane-2,4-diol



8-methylnonan-4-ol

Alcohol Group

More miscible (soluble) in water with more OH groups attached (hydrogen bonding)

Less miscible with longer hydrocarbon chains

Ether

Slightly soluble in water

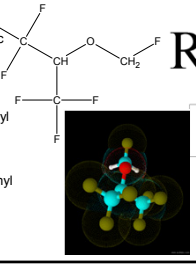
Common ethers:
diethylether (solvent, once used as anesthetic)
methyl tert-butyl ether (octane booster for gasoline)

Suffix: "ether"

Example of common anesthetic ether:
Sevoflurane (Ultane®)
$CHF_2OCH(CF_3)_2$
a.k.a.
fluoromethyl hexafluoroisopropyl ether

2,2,2-trifluoro-1-[trifluoromethyl]ethyl fluoromethyl ether

1,1,1,3,3,3-hexafluoro-2-(fluoromethoxy)propane



R—O—R'

Ether
ether

Amines

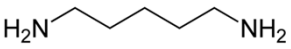
Alkyl substituted ammonia (One or more hydrogens on the nitrogen can be substituted)

Organic bases (react with acids to produce salts)

Can be primary, secondary or tertiary depending on how many hydrogens are substituted on the nitrogen

Usually offensive odors

Most not water soluble



Cadaverine or pentamethylenediamine is a toxic diamine produced during putrefaction of animal protein.

The molecular formula of cadaverine is $C_5H_{14}N_2$

Amine
-amine

Functional Groups Containing Carbonyl Group (-C=O)

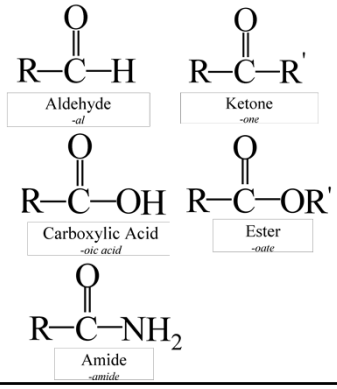
Aldehyde

Ketone

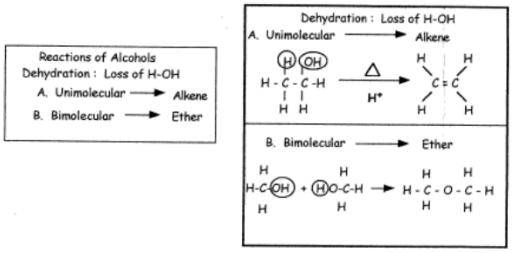
Carboxylic Acid

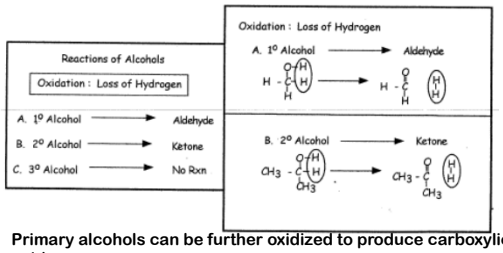
Esters

Amides



Alcohol Reactions





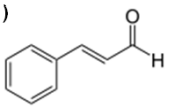
Primary alcohols can be further oxidized to produce carboxylic acids

These processes can be reversed by a reduction process

Common oxidizers: potassium permanganate, potassium dichromate
Common reducers: $NaBH_4$ (sodium borohydride or sodium tetrahydroborate), $LiAlH_4$ (lithium tetrahydroaluminate or lithium aluminum hydride), hydrogen gas H_2

Aldehydes and Ketones

Pleasant Odors
Seen in fragrances and flavorings (almond, cinnamon, raspberries)



Cinnamaldehyde
(2*E*)-3-phenylprop-2-enal

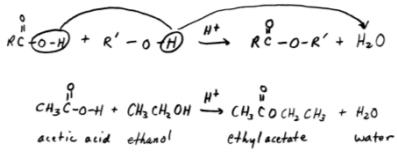
Carboxylic Acid

-Weak organic acid (H in the OH group dissociates)
-Component of ester production
-Acetic acid (ethanoic acid) one of the most widely used chemicals (made from oxidation of methanol or methanol + CO w/ catalyst

Esters

Generally pleasant odors

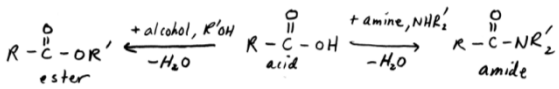
Esterification: The production of esters by reacting carboxylic acids with alcohols.



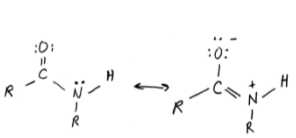
Ester + strong base –(heat/water)-> carboxylate salt + alcohol

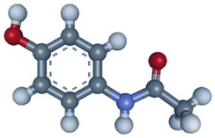
Carboxylate salt + strong acid ---> carboxylic acid and salt of strong acid

Amides



Resonance of amide to account for observed 120° bond angles of the nitrogen (instead of expected 109.5°)





Acetaminophen, N-acetyl-p-aminophenol

Polymers

Chains of monomers (base units) linked together

Can occur naturally (proteins, nucleic acids, etc.) or synthetically (nylon, polystyrene, etc.)

Two major types:

Addition polymers: Monomers directly linked together

Condensation polymers: Monomers liked together with the production of water (or other small molecule)

Copolymers = Formed from more than one type of monomer

Also: Polyesters and polyamides

Table 11.12 Ethylene Derivatives That Undergo Addition Polymerization

Formula	Monomer Common Name	Polymer Name (Trade Names)	Uses	U.S. Polymer Production (Metric tons/year)*
	ethylene	polyethylene (polythene)	squeeze bottles, bags, films, toys and molded objects, electric insulation	7 million
	propylene	polypropylene (Vectra, Herculon)	bottles, films, indoor-outdoor carpets	1.2 million
	vinyl chloride	polyvinyl chloride (PVC)	floor tile, raincoats, pipe	1.6 million
	acrylonitrile	polyacrylonitrile (Orlan, Acrilan)	rugs, fabrics	0.5 million
	styrene	polystyrene (Styrofoam, Styron)	food and drink coolers, building material insulation	0.9 million
	vinyl acetate	polyvinyl acetate (PVA)	latex paint, adhesives, textile coatings	200,000
	methyl methacrylate	polymethyl methacrylate (Plexiglass, Lucite)	high-quality transparent objects, latex paints, contact lenses	200,000
	tetrafluoroethylene	polytetrafluoroethylene (Teflon)	gaskets, insulation, bearings, pan coatings	6,000