Organic Chemistry

Introduction:
- this is the chemistry of compounds that contain covalently linked carbon atoms
- over 80% of the known chemicals are organic
- prior to 1820's organic molecules/compounds were isolated from animal and plant material
- Organic compounds are now defined as compounds that are based on carbo

The Carbon Atom
- carbon is a special element with the unique ability to bond together with many other carbon atoms, forming chains and rings
- usually form a total of 4 covalent bonds and therefore connect to as many as 4 other atoms
- form strong single, double, or triple bonds with other carbon atoms
- Carbon readily binds to other carbon atoms
  - called CATENATION
  - the carbon-carbon bonds are very hard to break, therefore organic molecules are very stable

Molecular Shape and Polarity:
- electronegativity is a measure of how strong an atom attracts electrons in a chemical bond
- in a polar covalent bond, the electrons are attracted more strongly to the atom with the higher EN
- thus, every polar bond has a bond-dipole: a partial negative charge and a partial positive charge, separated by the length of the bond

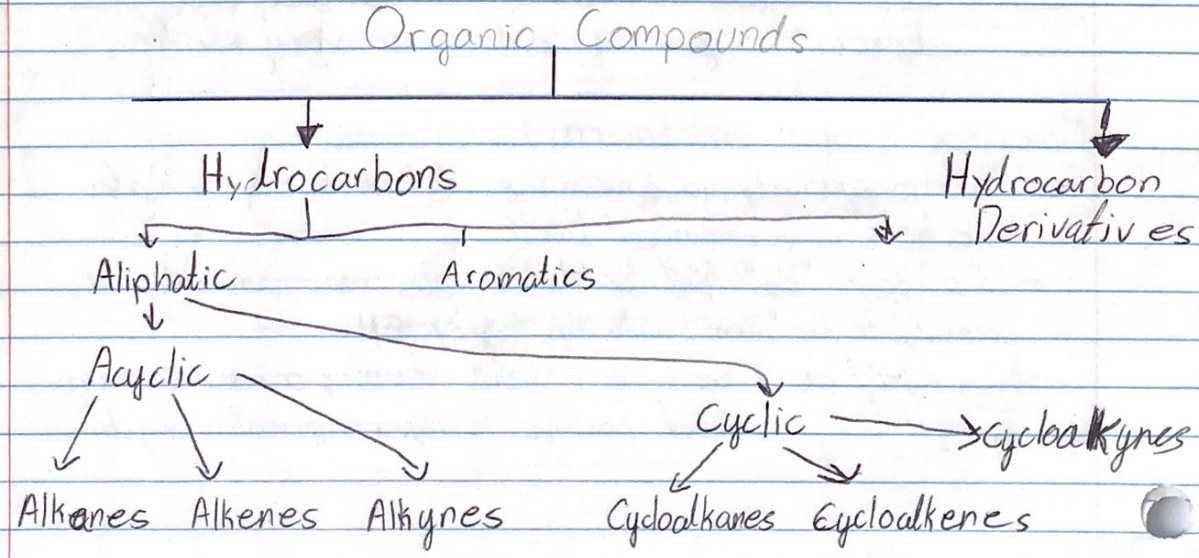
Hydrocarbons:

- compounds that only contain carbon and hydrogen atoms, thus are considered organic
- Examples of hydrocarbons:
  - fats and oils
  - coal and other petroleum products
  - the lipid layer of your cell membrane
  - soap

Prefixes for # of Carbons

#C	Prefix	#C	Prefix
1	Meth	6	Hex
2	Eth	7	Hept
3	Prop	8	Oct
4	But	9	Non
5	Pent	10	Dec

Classifaction of Hydrocarboms



Aliphatic Hydrocarbons

- organic compounds with molecular structures that are either straight, branched chains, or rings of C–C bonds
- compounds that are straight and branched are acyclic; rings are cyclic

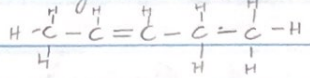
Aliphatic Families:

• Alkanes

- contains only single C–C bonds
- straight and branched have the formula: C_nH_{2n+2} (n = # of carbons)
- named ——ane
- ringed alkanes are called "cycloalkanes"
  - formula is: C_nH_{2n}
  - named cyclo——ane

• Alkenes

- alkenes have double bonds
- straight chain alkenes have the general formula: C_nH_{2n}
- named ——ene



• Alkynes

- Alkynes have triple bonds
- straight chain alkynes have the general formula: C_nH_{2n-2}
- named ——yne

Structural Diagrams:

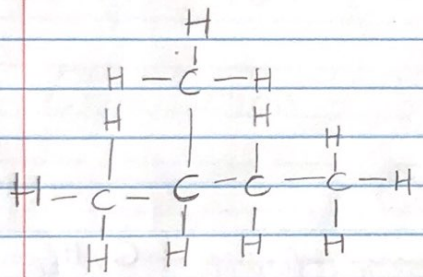
- three types of structural diagrams are used to depict organic molecules
  1. Complete Structural Diagram
  2. Condensed Structural Diagram
  3. Line Diagram

Ex:

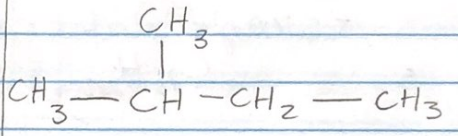
① Empirical Molecular Formula: C_5H_{12} ← alkane

② Expanded Molecular Formula: $CH_3\,CH(CH_3)\,CH_2\,CH_3$

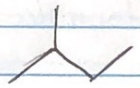
③ Structural Formula:



④ Condensed Structural Formula:



⑤ Line Structural Formula



Naming Side Chains:

Side Chain Length	Prefix Name	Side Chain Name	Alkyl Formula (C_nH_{2n+2-1})
1	meth	methyl	$-CH_4$
2	eth	ethyl	$-C_2H_5$
3	prop	propyl	$-C_3H_7$
4	but	butyl	$-C_4H_9$
5	pent	pentyl	$-C_5H_{11}$
6	hex	hexyl	$-C_6H_{13}$

Naming Alkanes:

Step 1:

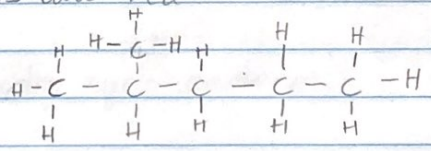
- find the longest chain
- if the chain is branched, the end of the longest chain closest to a branch is designated carbon 1.
- the remaining carbons in the longest chain are numbered as they appear

Step 2:

- Determine the number and types of branches
  - A hydrocarbon branch is called an Alkyl group
  - the branch is named for the Alkene it resembles with 2 differences
    - the name: -ane changes to -yl
    - the number of hydrogens decrease by one
  - Ex: ethane (C_2H_6) to ethyl ($-C_2H_5$)

Step 3:

- Designate the position of the branch by stating the # of the carbon in the longest chain it is attached
  - Ex: 2-methylpentane



Naming Alkenes and Alkynes:

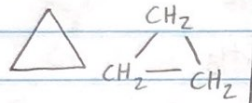
- IUPAC decided that the importance of the multiple bond play a central role in the naming of the alkenes and alkynes
- the longest parent chain must contain the multiple bond
- the numbering of the parent chain starts at the end closest to the multiple bond
- triple bonds are even more reactive than double bonds
- the name of the parent chain is preceded by a number that indicates the position of the multiple bond

Cyclic & Aromatic

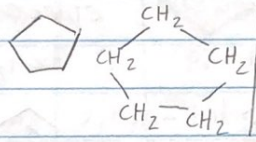
Cycloalkanes:

- are cyclic alkanes
- have two hydrogen atoms fewer than open chain
- are named by using the prefix cyclo- before the name of the alkene chain with the same number of carbon atoms
- the structural formulas of cycloalkanes are usually represented by shapes

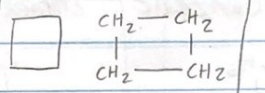
cyclopropane



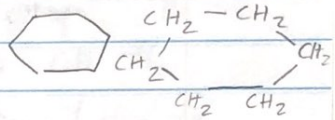
cyclopentane



cyclobutane

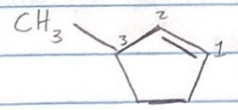


cyclohexane



Naming Cycloalkenes:

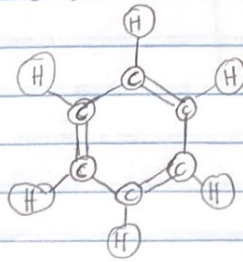
- cycloalkenes have a double bond within a ring structure and are named by assigning the double bond to be between Carbon 1 and Carbon 2 when a substituent is on the ring
- cycloalkenes have the general formula; C_nH_{2n-2}



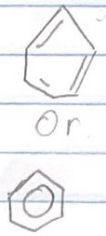
3-methy cyclo pentene

Aromatic Hydrocarbons:

- are organic compounds with rings of carbon bonded in alternating double-single-double structure that switch to single-double-single
- bonds are more stable than double bonds



or



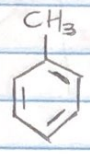
Aromatic Compounds

- Aromatic compounds contain benzene ring
- Benezene: C_6H_6
- some have a pleasant smell

Naming Aromatic Compounds

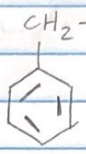
- benzene is the parent chain
- name of substituent comes in front of "Benzene"

methylbenzene



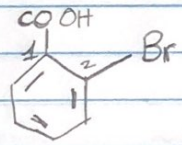
chlorobenzene

ethylbenzene

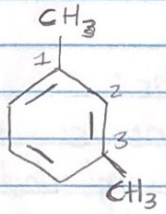


- when two groups are attached to benzene, the ring is numbered to give the lower numbers to the substituents

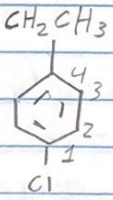
  - start numbering from a special name
  - if we do not have, number them to get the smallest set of #'s
  - list them by alphabetical order



2-bromobenzoic acid
Ortho-substituents are next to each other



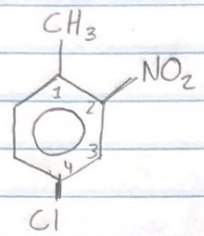
1,3-Dimethylbenzene



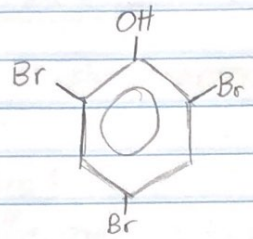
1-Chloro-4-ethylbenzene

Naming of Aromatic Compounds (cont):

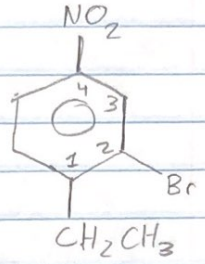
- if we have three or more substituents:
  - start numbering from special name (if we have)
  - if we do not have, number them to get the smallest set of numbers
  - list them by alphabetical order



4-Chloro-2-Nitrotoluene



2,4,6-tribromophenol



2-Bromo-1ethyl-4-nitrobenzene

Isomers

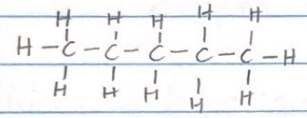
What are Isomers:

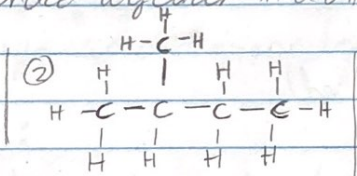
- Molecules that have the same molecular formula but their atoms are in a different arrangement

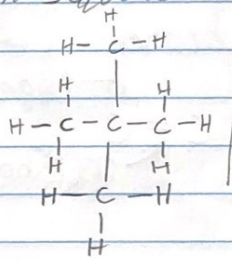
Isomers
- constitutional isomers
- stereoisomers

Constitutional Isomers:

- molecules that have the same molecular formula, but their atoms are bonded together in a different sequence

① 

② 

③ 

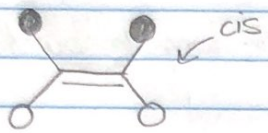
all are C_5H_{12}

Stereoisomers:

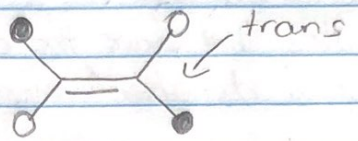
- molecules that have the same molecular formula and their atoms are bonded together in the same sequence, but differ in the 3-dimensional orientations of their atoms in space
- an important property of this molecule is that it cannot rotate around the double bond. Therefore, the molecule is flat & rigid

Stereoisomers
- Diastereomers
  - cis/trans isomers
- Enantiomers

Stereochemical Notation:



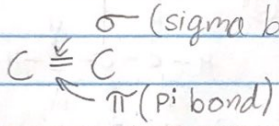
identical substituents on the same side



identical substituents on opposite sides

* Stereoisomers based on double bonds are called DIASTEREOMERS

* interconversion of stereoisomeric alkenes does not normally occur. It requires that the π component of double bond be broken



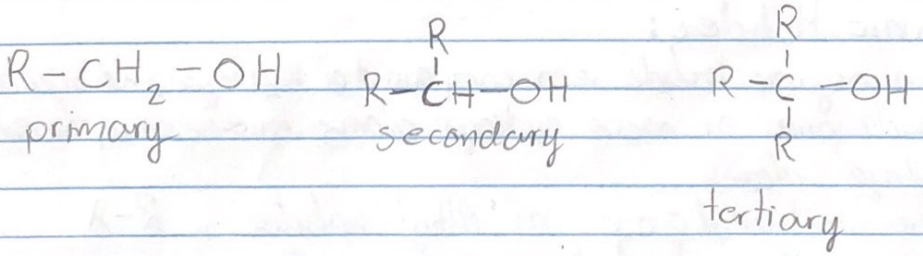
Alcohols and Haloalkanes

Functional Groups:
- are a useful way to classify organic compounds
  1. compounds with the same functional group often have similar physical properties
  2. compounds with the same functional grouph react chemically in very similar ways

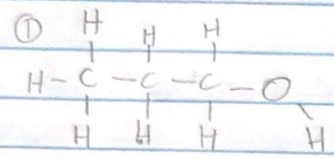
Alcohols:
- an organic compound characterized by the presence of a hydroxyl group; R-OH
- depending on the position of the hydroxyl group, an alcohol can be primary, secondary, or tertiary

Naming Alcohols:
1. Locate the largest chain that contains an OH grap Name the parent alkane
2. Replace the -e at the end of the parent alkane name with -ol
3. Add a position number for location of -OH group
4. Name and number the branches

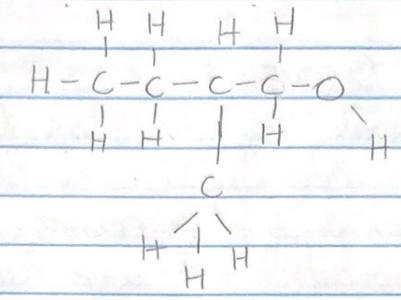
***
- Alcohols are classified based on how many carbon are attached to the C-OH



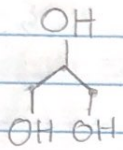
Ex:

① 

propanol

② 

2-methyl butanol

③ 

← propane-1,2,3-triol

Properties of Alcohols:

- Alcohols are polar but strength decreases with increased size
- Most are liquids at room temperature
- the H-bond and small alcohols are extremely soluble in water solubility decreases with size
- Alcohols have higher MP and BP than Alkanes
- they are mainly used as solvents, antiseptics, and components of antifreeze
- they are extremely flammable and poisonous, often causing blindness, impairment, and death

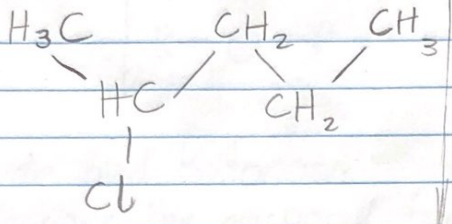
Organic Halides:

- an organic halide is a compound of hydrogen and carbon in which one or more hydrogen atoms have been replaced by halogen atoms
- the functional group of Alkyl halides is R-X where X represents a halogen atom

Naming Alkyl Halides:
- follow alkane rules and add position numbers and prefixes fluoro, chloro, bromo, or iodo.

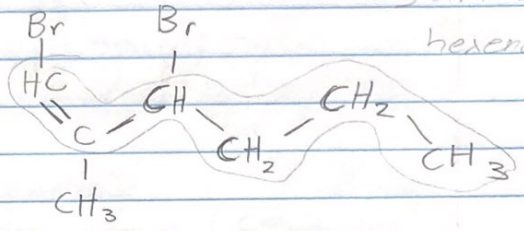
- branches and halides have equal priority
- number the carbons alphabetically
- double bonds have higher priority than halides

Ex:



2-chloro pentane

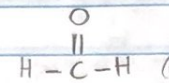
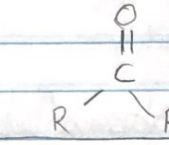
1,3-dibromo



1,3-dibromo-2methylhexene

Aldehydes, Ketones, Ethers

Functional Groups:

Aldehyde	 (formyl group)	-al
Ketone	 (a carbonyl group)	-one
Ether	R—O—R' (alkoxy group)	-oxy ; -yl

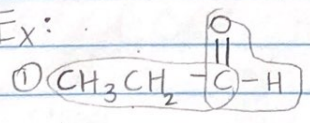
Aldehyde and Ketones:
- both have the carbonyl function group (C=O)

- aldehydes have a strong pungent smell, while ketones smell sweet
- aldehydes with higher molecular masses have a pleasent smell

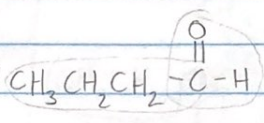
Aldehydes:
- an aldehyde is an organic compound that has a double-bonded oxygen on the last/first carbon of a carbon chain
- the general formula is R-CHO

How to Name an Aldehyde:
1. Name the parent alkane, the carbon atom of the carbonyl group is position 1
2. Replace the -e at the end of the parent alkane with -al

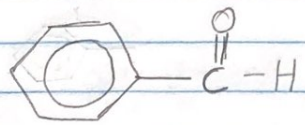
Ex:



① propyl

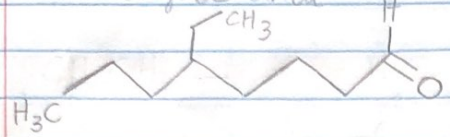


② butanyl

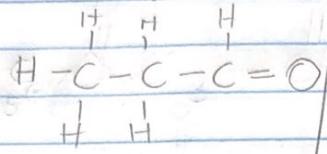


③ benzaldehyde

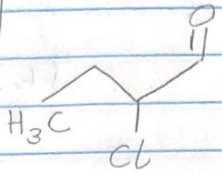
5-ethyl octanal



propanyl



2-chlorobutanal



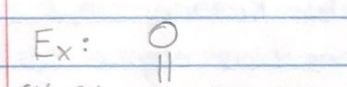
Ketones:

- a ketone is an organic compound that has a double-bonded oxygen on any carbon within the carbon chain
- the general formula for a ketone is RCOR'

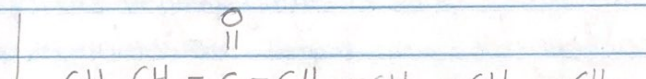
How to Name a Ketone:

- name the parent alkane
- replace -e at the end with -one

Ex:

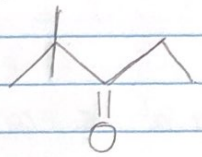


pentan-3-one

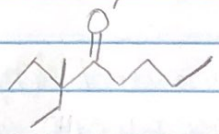


heptan-3-one

2,2-dimethylpentan-3-one

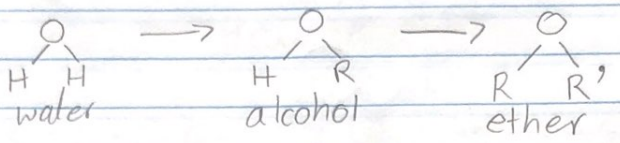


3-ethyl-3 methyl octan-4-one



Ethers:

- an ether is an organic compound with two alkyl groups attached to an oxygen atom



- the general formula is R-O-R
- ethers are extremely flammable

How to Name Ethers:

1. Choose the longest alkyl group as the parent alkane
2. Treat the second alkyl group, along with the oxygen atom as an alkyl group. Name it by replacing the -yl ending with -oxy
3. Put the prefix and suffix together: alkoxy group + parent alkane

How to Name Ethers (common name):

1. list alkyl groups in alphabetical order
2. place the suffix -ether at the end of the name

Ex: $CH_3-CH_2-O-CH_2-CH_2-CH_3$

CH_3-CH_2: ethyl → ethoxy

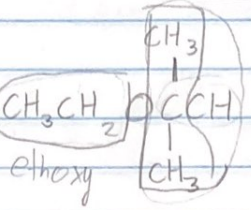
$CH_2-CH_2-CH_3$: longest alkyl group → 3 C's (propane)

1-ethoxy propane or ethyl propyl ether

$CH_3CH_2OCH_2CH_3$

ethyl → ethoxy; ethyl → ethane

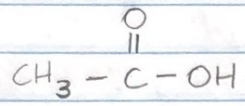
ethoxy ethane
or diethyl ether



2-ethoxy 2-methyl propane

Carboxylic Acids & Esters

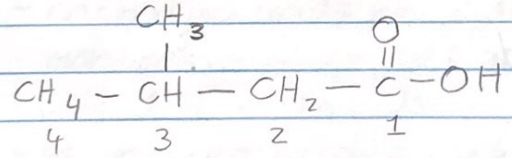
Carboxylic Acid:
- contains a carboxyl group, which is a carbonyl group (C=O) attached to a hydroxyl group (-OH)
- has the carboxyl group (-COOH) on carbon 1



IUPAC Naming:
- replace the -e in the alkane name with -oic acid

- CH_4 (methane) — $HCOOH$ ← methanoic acid
- CH_3-CH_3 (ethane) — CH_3-COOH ethanoic acid

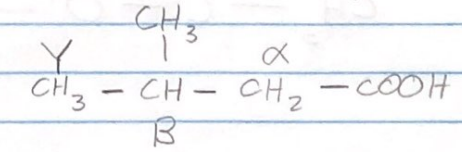
- Number substituents from the carboxyl carbon 1



Common Names:

1 Carbon	formic acid
2 Carbon	acetic acid
3 Carbon	propionic acid
4 Carbon	butyric acid

*locate substituents using γ, β, α



3-methylbutanoic acid
or β-methylbutyric acid

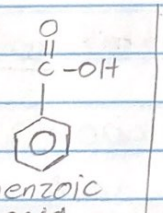
Alpha hydroxy acids:

- occur naturally in fruit, milk, and sugarcane
- used in skin care products

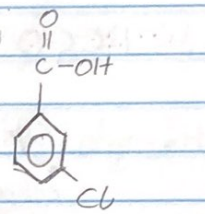
Aromatic Carboxylic Acids:

- Benzoic Acid
  - is the aromatic carboxylic acid
  - locate substituents by assigning 1 to the carbon attached to the carboxyl group
  - has common names that assign prefixes 'ortho', 'meta', and 'para' for 2 substituents

***	
ortho	1, 2
meta	1, 3
para	1, 4

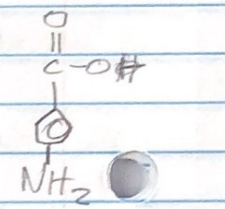


benzoic acid



3-chlorobenzoic acid

m-chlorobenzoic acid

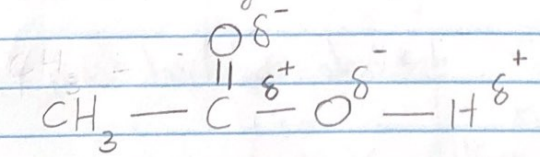


4-aminobenzoic

p-aminobenzoic

Polarity of Carboxylic Acids:

- are strongly polar
- have two polar groups:
  1. hydroxyl (-OH)
  2. carbonyl (C=O)



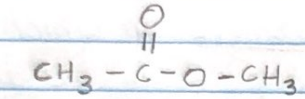
- The boiling points of carboxylic acids:
  - are higher than alcohols, ketones, and aldehydes of similar mass
  - are high because they form <u>dimers</u> in which hydrogen bonds form between the polar groups in the two carboxyl groups

Compound	Molar Mass	Boiling Point
$CH_3-CH_2-\overset{\overset{O}{\|\|}}{C}-H$	58	49°C
$CH_3-CH_2-CH_2-OH$	60	97°C
$CH_3-\overset{\overset{O}{\|\|}}{C}-OH$	60	118°C

Solubility in Water:
- carboxylic acids for hydrogen bonds with many water molecules
- with 1-4 carbon atoms are very soluble in water
- as you increase, boiling point also increases, and solubility in water decreases

Esters:

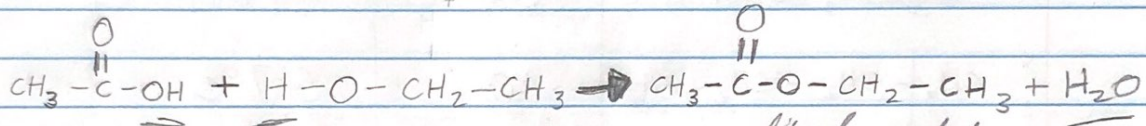
- In an ester:
  - the H in the carboxyl group is replaced with an alkyl group



ester group

Esterfication:

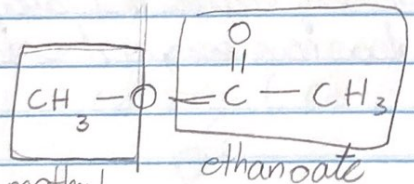
- the reaction of a carboxylic acid and alcohol in the presence of an acid catalyst to produce an ester



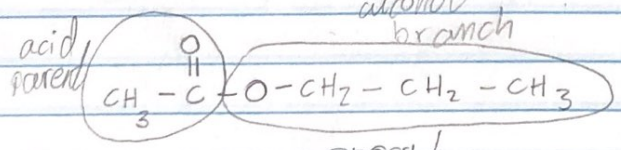
ethyl acetate
ethyl ethanoate

Naming Esters:

- The name of an ester contains the names of
  - the alkyl group from the alcohol
  - the carbon chain from the acid with -ate ending



methyl ethanoate

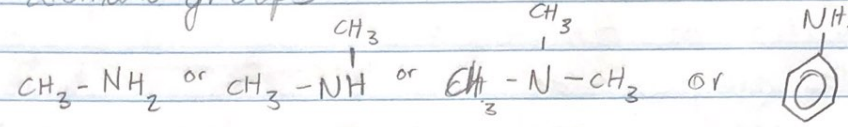


acid parent
alcohol branch
propyl

ethyl ethanoate ∴ propyl ethanoate

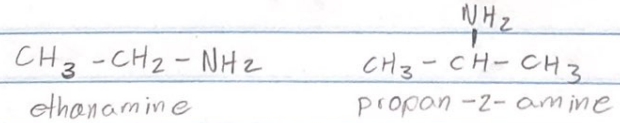
Amines and Amides

Amines:
- are derivatives of ammonia NH_3
- contains N attached to one or more alkyl or aromatic groups



Classification of Amines:
- Amines are classified as primary, secondary, or tertiary
  - in a primary (1°) amine, 1 C group is bonded to N
  - in a secondary (2°) amine, the amine has 2 carbon groups
  - a tertiary (3°) amine has 3 Carbon groups

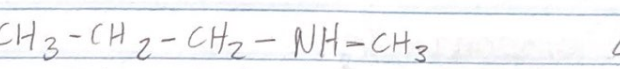
IUPAC Names of Amines:
- amines are named as alkanamines
- the "e" in the alkane name of the longest changed to amine
- the chain is numbered to locate the amine group and substituents



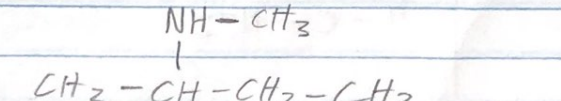
ethanamine

propan-2-amine

Naming Secondary & Tertiary Amines:
- the longest alkane chain is numbered
- each alkyl group bonded to the N atom is named as a N-alkyl group



N-methylpropan-1-amine



N-methylbutan-2-amine

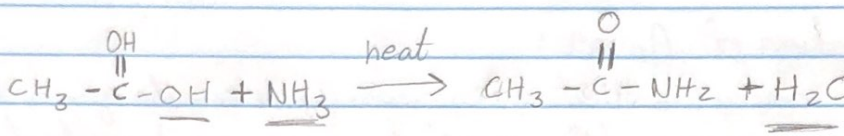
Boiling Points of Amines

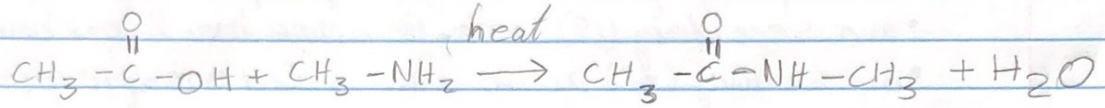
- the BP of amines are:
  1. higher than alkanes
  2. lower than alcohols of similar mass

Amides

Preparation of Amides:

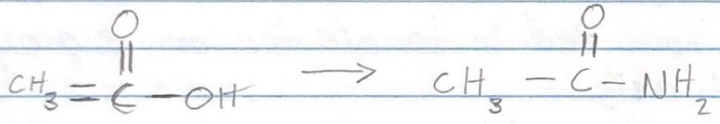
* Amides are prepared
  - by reacting a carboxylic acid with ammonia or amine (1° or 2°)





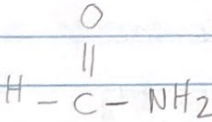
Amides:

- In amides, an amino group ($-NH_2$) replaces the $-OH$ group of carboxylic acids

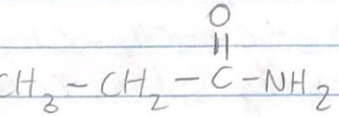


Naming Amides

- Amides are named as alkanamides
- replace -oic acid ending with -amide



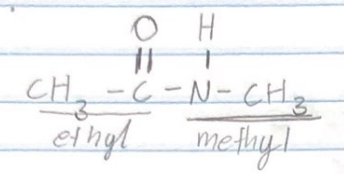
methanamide



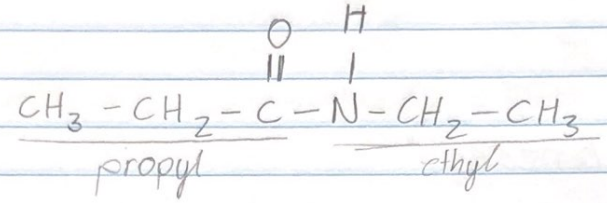
propanamide

Amides With N-Groups

- An alkyl group bonded to an N atom is named as N-alkyl infront of the amide name



N-methyl ethanamide



N-ethyl propan amide

Properties:

Amides...

- that are primary ($-NH_2$) or secondary ($-NH-$) form H-bonds
- that are primary have higher melting points than secondary
- that are tertiary do not form H-bonds and have lower melting points