INTRODUCTION to FUNCTIONAL groups

- It is useful to view a molecule as being composed of two parts. One part only has C's that are singly bonded to other C's (and their associated H's)
- This group of atoms is called the alkyl group, the carbon skeleton, or the carbon framework and has little effect on the chemical reactions

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- The other part of the molecule, where the action is, is called the functional group. There is an entire new set of chemical reactions for each new compound encountered.
- A particular arrangement or group of atoms has very similar chemistry no matter what the remainder of the molecule looks like.

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Common functional groups

- Alkanes, R-H (and cycloalkanes)
- Alkenes, RCH=CHR
- Alkynes, R-CΞC-R
- Alcohols, R-OH
- Aldehydes, RCHO
- Alkyl halides, R-X (X=F, Cl, Br,I)
- Amines, R-NH_2
- Aromatics, Ar-H

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Common functional groups

- Carboxylic Acids, RCOOH
- Carboxylic Acid Derivatives:
  - Acid Anhydride, RCOOCOR'
  - Amide, $RCONH_2$
  - Acid Chloride, RCOCl
  - Ester, RCOOR'
- Ether, ROR'
- Ketones, RCOR'
- Nitriles, RCΞN

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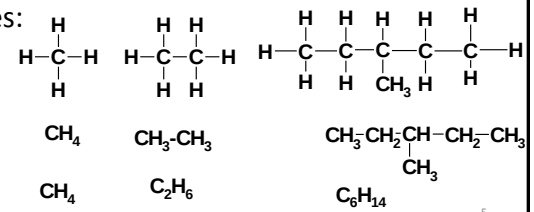
Alkanes

- Strictly speaking, alkanes do not have any functional groups as they form the basic skeleton on which the functional groups are attached.
- General formula: C_nH_{2n+2}
- Examples:



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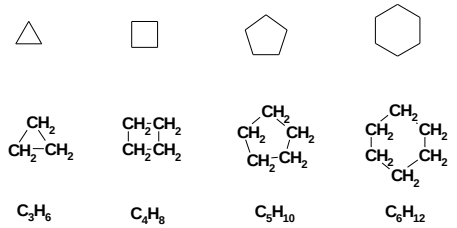
Cycloalkanes

- These are alkanes which exist in a ring
- General formula, C_nH_{2n}
- Examples



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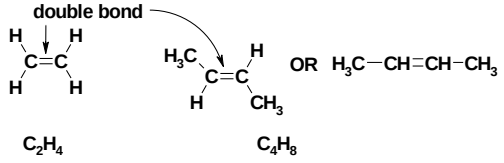
Alkenes

- The functional group is the double bond
- General formula: C_nH_{2n}
- The simplest alkene has 2 carbon atoms
- Examples



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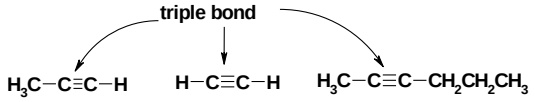
Alkynes

- The functional group is the triple bond
- General formula: C_nH_{2n-2}
- Examples:



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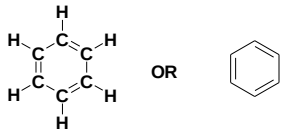
Aromatics

- These are a special type of alkenes which have 3 double bonds in a ring.
- The properties are different from normal alkenes so they are studied differently
- Examples:



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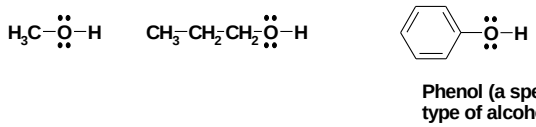
Alcohols

- The functional group is an OH
- General formula, R-OH
- Alcohols are related to water, H-O-H (H_2O)
- Examples



Phenol (a special type of alcohol)

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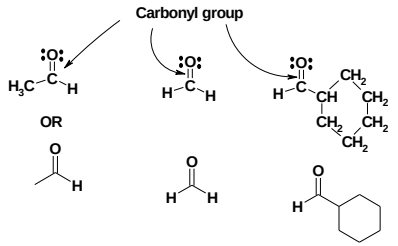
Aldehydes

- The functional group is carbonyl group (C=O) attached to a hydrogen atom
- General formula, RHC=O
- Examples



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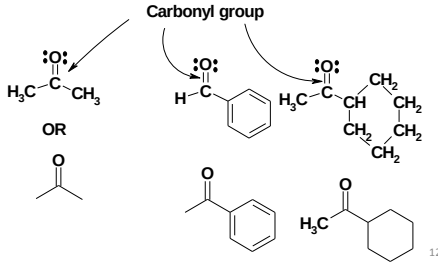
Ketones

- The functional group is carbonyl group (C=O) attached to an alkyl or an aromatic group
- General formula, $R_2C=O$
- Examples



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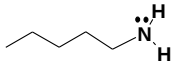
Amines

- The functional group is the amino (NH_2) group
- General formula, RNH_2
- Examples

CH_3-NH_2



CH_3–CH_2–CH_2–CH_2–CH_2–NH_2

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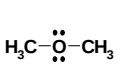
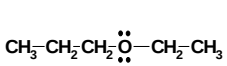
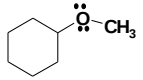
Ethers

- The functional group is the oxygen atom between two alkyl groups
- The general formula is ROR
- Examples







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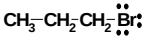
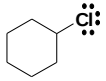
Alkyl halides

- The functional group is the halogen atom
- The general formula is RX where X = F, Cl, Br or I
- Examples





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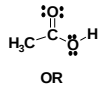
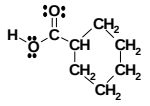
Carboxylic acid

- The functional group is carbonyl acid group (C=O) attached to a hydroxyl group
- General formula, RCOOH
- Examples



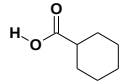
OR

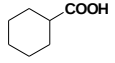


OR

CH3COOH

HCOOH





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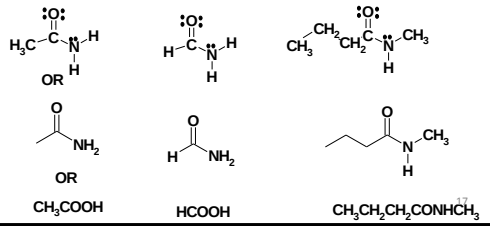
Amide (a Carboxylic Acid Derivative)

- This compound is derived from carboxylic acid
- General formula, $RCONH_2$
- All carboxylic acid derivatives contain the carbonyl group (C=O).
- Examples



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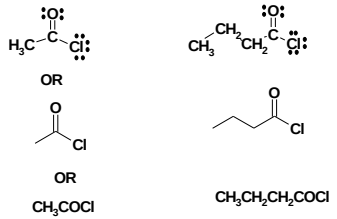
Acid Chloride (a Carboxylic Acid Derivative)

- This compound is derived from carboxylic acid
- General formula, RCOCl
- Examples



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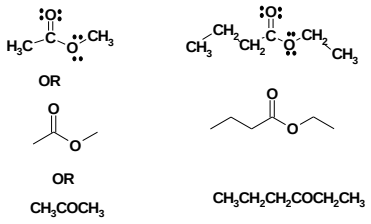
Ester (a Carboxylic Acid Derivative)

- This compound is derived from carboxylic acid
- General formula, RCOOR'
- Sometimes the R and R' groups are the same
- Examples



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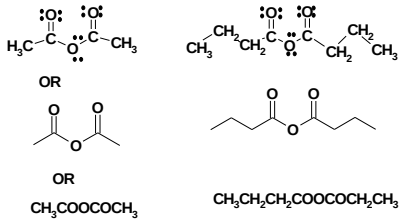
Acid Anhydride (a Carboxylic Acid Derivative)

- This compound is derived from carboxylic acid
- General formula, RCOOCOR'
- Sometimes the R and R' groups are the same
- Examples



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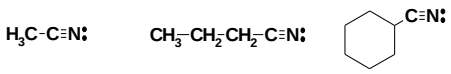
Nitriles

- The functional group is the carbon-nitrogen triple bond
- The general formula is RC≡N
- Examples



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Note

- The names of certain functional groups changes when they are part of a more complex molecule. For example:

Group	Parent	substituent
OH	Alcohol	hydroxyl
C=O	Ketone/Aldehyde	carbonyl
C≡N	Cyanide	nitrile
C=C	Alkene	Double bond
	Benzene	Phenyl/ Aryl

- The next slide shows the molecule - Rapamycin

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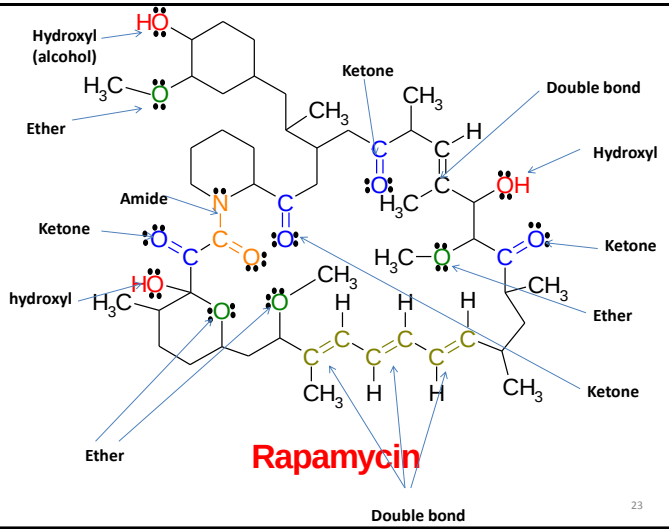

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Frequency of functional groups

Group	Frequency
Hydroxyl (alcohol)	3
Ketone	3
Double bond	4
Ether	4
Amide	1

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IUPAC nomenclature of organic chemistry

The steps to naming an organic compound are:

- Identify the parent hydrocarbon chain.
- This chain must follow the following rules, in order of precedence:
  - It should have maximum substituents of the suffix functional group. By suffix, it is meant that the parent functional group should have a suffix, unlike halogen substituents. If more than one functional group is present, use the one with highest precedence.
  - It should have maximum number of multiple bonds
  - It should have maximum number of double bonds.
  - It should have the maximum length.

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IUPAC nomenclature of organic chemistry

- Identify the parent functional group, if any, with the highest order of precedence.
- Identify the side-chains. *Side chains are the carbon chains that are not in the parent chain, but are branched off from it.*
- Identify the remaining functional groups, if any, and name them by the name of their ions (such as hydroxy for -OH, oxy for =O , oxyalkane for O-R, etc.).

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IUPAC nomenclature of organic chemistry

- Number the chain. To number the chain, first number in both directions (left to right and right to left), and then choose the numbering which follows these rules, in order of precedence:
  - Has the lowest locant (or locants) for the suffix functional group. Locants are the numbers on the carbons to which the substituent is directly attached.
  - Has the lowest locants for multiple bonds (The locant of a multiple bond is the number of the adjacent carbon with a lower number).
  - Has the lowest locants for double bonds
  - Has the lowest locants for prefixes.

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IUPAC nomenclature of organic chemistry

- Number the various substituents and bonds with their locants. If there is more than one of the same type of substituent/double bond, add the prefix (di-, tri-, etc.) before it. The numbers for that type of side chain will be grouped in ascending order and written before the name of the side-chain. If there are two side-chains with the same alpha carbon, the number will be written twice. Example: 2,2,3-trimethyl- .
- If there are both double bonds and triple bonds, write the "ene" before the "yne".

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IUPAC nomenclature of organic chemistry

- In case the main functional group is a terminal functional group (A group which can only exist at the end of a chain, like formyl and carboxyl groups), there is no need to number it.
- Add punctuation: Put commas between numbers (2 5 5 becomes 2,5,5)
- Put a hyphen between a number and a letter (2 5 5 trimethylheptane becomes 2,5,5-trimethylheptane)
- Successive words are merged into one word (trimethyl heptane becomes trimethylheptane)
  Note: IUPAC uses one-word names throughout. This is why all parts are connected.

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Order of precedence of groups

- When compounds contain more than one functional group, the order of precedence determines which groups are named with prefix or suffix forms.
- The highest precedence group takes the suffix, with all others taking the prefix form.
- However, double and triple bonds only take suffix form (-en and -yn) and are used with other suffixes.

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Order of precedence of groups

- Prefixed substituents are ordered alphabetically (excluding any modifiers such as di-, tri-, etc.),
- If there are multiple functional groups of the same type, either prefixed or suffixed, the position numbers are ordered numerically
- The *N* position indicator for amines and amides comes before "1", e.g. $CH_3CH(CH_3)CH_2CH_2NH(CH_3)$ is *N*,2-dimethylbutanamine.

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Order of precedence of groups

Priority	Functional group	Formula	Prefix	Suffix
1	Carboxylic acids	–COOH	carboxy-	-oic acid*
2	*Carboxylic acid derivatives:* Esters Acyl halides Amides	 –COOR –COX $–CONH_2$	 R-oxycarbonyl- halocarbonyl- carbamoyl-	 -R-oate -oyl halide* -amide*
3	Nitriles	-CN	cyano-	-nitrile*
4	Aldehydes	–CHO	formyl-	-al*
5	Ketones	C=O	Oxo-	-one
6	Alcohol	-OH	hydroxy-	-ol
7	Amines	$-NH_2$	Amino-	-amine
8	Alkenes and Alkynes: Alkene > alkyne	-C=C -C C-	**Chain numbering starts from the end closest to either group, unless they're both equidistant from the chain ends, in which case the *double bond takes***	substances containing double and triple bonds are called ***alkenynes***

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