Intro to Organic Chemistry: A summary

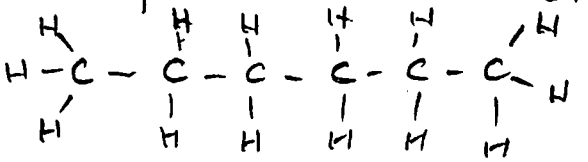
Hydrocarbons

As the name implies, those are compounds of carbon and hydrogen only.

* Alkanes

Only single bonds between carbons.

Carbons form a chain like:

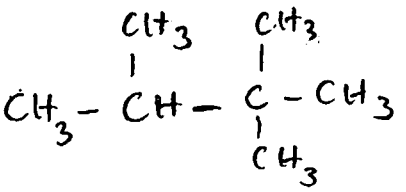


or $CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$

or more generally

$$CH_3-(CH_2)_n-CH_3$$

or they can be branched like:



But the general empirical formula of alkanes is:

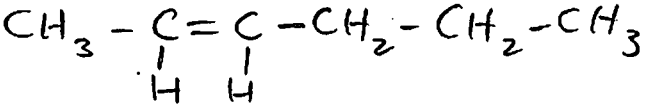
$$C_nH_{2n+2}$$

* Alkenes

Can have one or more double bonds between carbons. Each double bond reduces the number of hydrogens by 2

So, for alkenes with one double bond, the general empirical formula is

$$C_nH_{2n}$$

Example: 

Alkynes

* Can have one or more triple bonds between carbons
Each triple bond reduces the number of hydrogens by 4.
So, alkynes with one triple bond, the empirical formula is

$$C_nH_{2n-2}$$

Example: $H-C\equiv C-CH_2-CH_3$

Names of alkenes and alkynes derive from the names of alkanes with the same number of carbons.

# of carbons	Alkane		Alkene (one C=C)		Alkyne (one C≡C)	
	Formula	Name	Formula	Name	Formula	Name
1	CH_4	methane	—	—	—	—
2	C_2H_6	ethane	C_2H_4	ethene	C_2H_2	ethyne
3	C_3H_8	propane	C_3H_6	propene	C_3H_4	propyne
4	C_4H_{10}	butane	C_4H_8	butene	C_4H_6	butyne
5	C_5H_{12}	pentane	C_5H_{10}	pentene	C_5H_8	pentyne
6	C_6H_{14}	hexane	C_6H_{12}	hexene	C_6H_{10}	hexyne
7	C_7H_{16}	heptane	C_7H_{14}	heptene	C_7H_{12}	heptyne
8	C_8H_{18}	octane	C_8H_{16}	octene	C_8H_{14}	octyne
9	C_9H_{20}	nonane	C_9H_{18}	nonene	C_9H_{16}	nonyne
10	$C_{10}H_{22}$	decane	$C_{10}H_{20}$	decene	$C_{10}H_{18}$	decyne

Substitutions

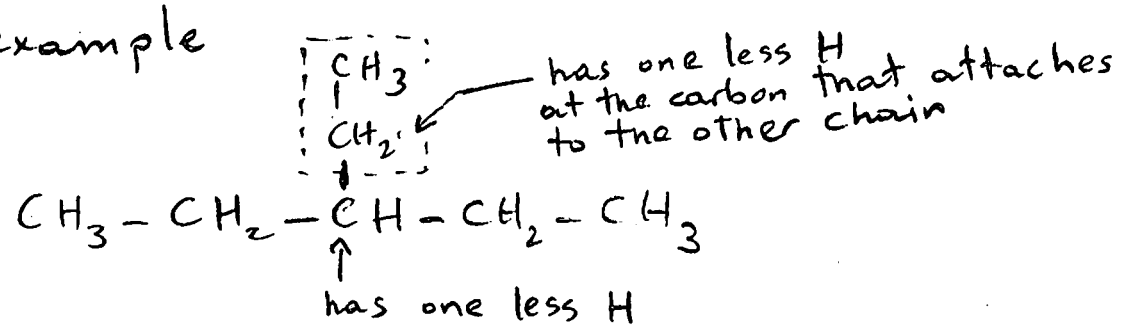
Straight chain alkanes are called "normal", and their names are prefixed with "n-"

For example:

$CH_3-CH_2-CH_2-CH_2-CH_3$ n-pentane

Branched alkanes are obtained when one or more hydrogens in the chain are substituted by shorter alkane chains. Just as the carbon where substitution occurs must lose one hydrogen to make room for the substituent, the shorter alkane chain taking the place of the hydrogen must come with a missing hydrogen as well in order to make the C-C bond with the carbon on the main chain.

For example

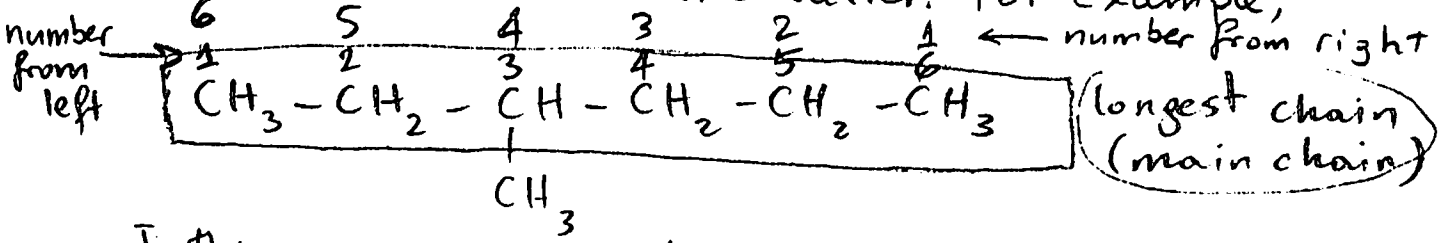


In the above example, CH_3-CH_2- is an "alkyl" group, specifically an "ethyl" group. When alkane chains act as substituent groups, the -ane at the end of their names is replaced with -yl. Therefore

CH_3-	methyl
C_2H_5-	ethyl
C_3H_7-	propyl
C_4H_9-	butyl
$C_5H_{11}-$	pentyl

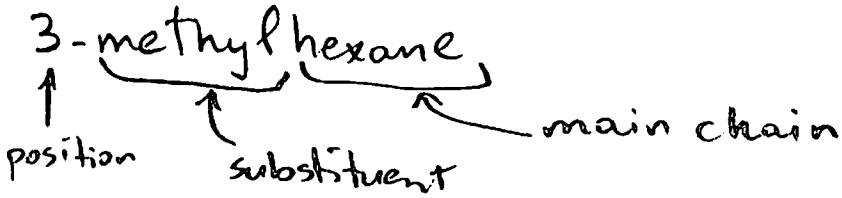
etc.

When naming alkanes with substituents, we first find the longest chain of carbon atoms and declare that as the "main chain" of the alkane, and the other branches are alkyl substituents. We also need to indicate which carbons on the main chain have substitutions. We number the carbon atoms starting from one of the two ends of the main chain. Whichever end makes the number of the first carbon that has a substitution smaller. For example,

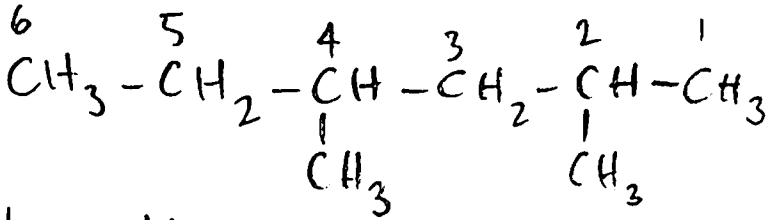


In this case we number the main chain carbons from the left, because that makes the CH_3- (methyl) substitution site to be "3", rather than "4".

The main chain has six carbons, so it is hexane, and it has a methyl group at C-3 (third carbon). Its name would then be:



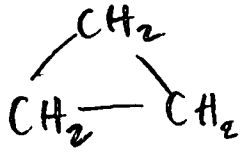
On the other hand, if we had the following structure:



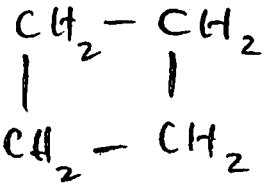
it would be named 2,4-dimethylhexane

Cyclic alkanes

If an alkane chain connects back to itself, it forms a cyclic alkane, and is named similarly to normal alkanes, except its name is prefixed with "cyclo"



cyclopropane



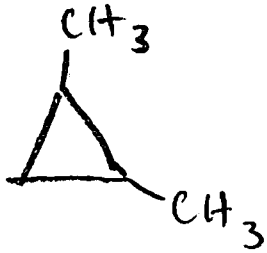
cyclobutane

etc.

We often draw the cyclic structures without showing the carbons or hydrogens, and only show the substituents

cyclopropane

methylcyclopropane



1,2-dimethylcyclopropane

Naming alkenes and alkynes

For main chains with up to 3 carbons, there is no ambiguity about the location of the C=C or C≡C bond; it has to involve a carbon that is at one end of the chain. For longer chains, we need to indicate the location of the double or triple bond by numbering the carbons from the end that minimizes the position number of the first carbon involved in a double or triple bond.

$CH_2=CH-CH_2-CH_3$ 1-butene

$CH_3-CH=CH-CH_3$ 2-butene

2-butene: "2" indicates position of C=C; "butene" indicates C=C

Let's throw in a substituent:

$CH_3-CH=C(CH_3)-CH_3$ 2-methyl-2-butene

$CH_3-CH_2-C\equiv C-CH(CH_2-CH_3)-CH_2-CH_3$; main chain

carbon #3 (rather than 5, because it's part of the main chain, and its position number gets minimized)

CH_2-CH_3 } ethyl (substituted at C-5 because C≡C dictated the numbering scheme to be from the left)

5-ethyl-3-heptyne

Addition reactions of alkenes and alkynes

When H_2 or X_2 (where X is a halogen, often Br_2) is added to "unsaturated" hydrocarbons (alkenes and alkynes), the π-bonds of the C=C or C≡C get broken and form σ-bonds with H or X

$$CH_2{=}CH{-}CH_3 + H_2 \longrightarrow CH_3CH_2CH_3$$

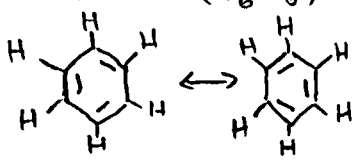
"unsaturated" → "saturated"

$$CH_2{=}CH_2 + Br_2 \longrightarrow CH_2Br{-}CH_2Br$$

Aromatic Hydrocarbons

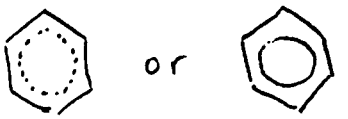
Cyclic hydrocarbons with π-bonds placed in such a way that allows the π-electrons to be delocalized over the entire ring.

The smallest and most common aromatic (and neutral) molecule is benzene (C_6H_6):



resonance forms of benzene

π-bonds are delocalized:



(hydrogens not shown)

Aromatic rings have extra stability due to delocalization (aromaticity).

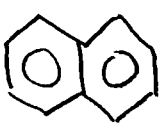
If the ring has resonance structures with alternating double and single bonds all around the ring, it is aromatic, or has "aromaticity".

Aromaticity requires $4n+2$ π-electrons (and an equal number of carbon atoms if the ring is neutral and is composed of C atoms)

Benzene has $4(1)+2 = 6$ carbon atoms

The next aromatic ring has $4(2)+2 = 10$ carbon atoms

Generally, aromaticity is achieved by joining 6-membered rings, such as in naphthalene:



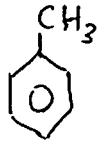
naphthalene has 10 carbons with 10 π-electrons (5 π-bonds)

Aromatic molecules are planar (sp^2 hybridized carbons connected together).

Naming benzene derivatives:

One substituent:

— Similar to other hydrocarbons

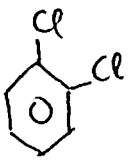


methylbenzene (common name: toluene)

chlorobenzene

Two substituents:

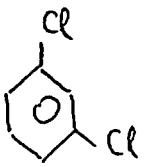
— Standard name similar to other alkenes



1,2-dichlorobenzene
ortho-dichlorobenzene

* Common naming scheme involves ortho-, meta-, para- prefixes

substituents on neighboring C's



1,3-dichlorobenzene
meta-dichlorobenzene

substituents on C's separated by one C.

1,4-dichlorobenzene
para-dichlorobenzene

substituents on C's separated by two C's

Non-hydrocarbons

When we have non-hydrocarbon substitutents on the hydrocarbon chain, we no longer have a hydrocarbon. The nature and the naming of the compound is now different. The hydrocarbon part itself is viewed as a "substituent" (generally denoted as R- or R'- etc.) The naming, properties and reactions revolve around the non-hydrocarbon "functional group".

Class	Functional group	General formula	Example	
Halohydrocarbons	$-X$ (F, Cl, Br, I)	$R-X$	CH_3I	iodomethane
Alcohols	$-OH$	$R-OH$	CH_3OH	methanol
Ethers	$-O-$	$R-O-R'$	CH_3OCH_3	dimethyl ether
Aldehydes	$-\overset{O}{\overset{\|}{C}}-H$	$R-\overset{O}{\overset{\|}{C}}-H$	$H-\overset{O}{\overset{\|}{C}}-H$	methanal
Ketones	$-\overset{O}{\overset{\|}{C}}-$	$R-\overset{O}{\overset{\|}{C}}-R'$	$CH_3-\overset{O}{\overset{\|}{C}}-CH_3$	dimethyl ketone
Carboxylic acids	$-\overset{O}{\overset{\|}{C}}-OH$	$R-\overset{O}{\overset{\|}{C}}-OH$	$CH_3-\overset{O}{\overset{\|}{C}}-OH$	ethanoic acid (acetic acid)
Esters	$-\overset{O}{\overset{\|}{C}}-O-$	$R-\overset{O}{\overset{\|}{C}}-O-R'$	$CH_3-\overset{O}{\overset{\|}{C}}-O-CH_2CH_3$ (acetate (anion of acetic acid); ethyl)	ethyl acetate (ethyl ethanoate)
Amines	$-NH_2$	$R-NH_2$	CH_3NH_2	methylamine