IUPAC Rules for nomenclature

From your previous studies, you should have covered the basics of naming. This document will summarise the key concepts you are required to know to name molecules in 1st year. Some parts of this will be brief and other more common problematic areas will be covered in slightly more detail.

Why do we need a systematic naming configuration?

A standardised naming system was introduced by IUPAC (International Union of Pure and Applied Chemistry) to eliminate ambiguity in the names of compounds and molecules. Before this, chemists around the world would refer to the same molecule or compound with different names which led to confusion amongst chemists from different parts of the world. The IUPAC standard of naming ensures that a certain compound or molecule has one name that is recognised internationally by all chemists.

The IUPAC naming convention treats names as 'formulas' which are built up based on the structure of the molecule. Rather than each molecule having a fixed name that must be memorised, the name of a molecule is created using simple rules. It must be emphasized that the rules of naming are not difficult (although it may seem like it at first glance); put it this way, if IUPAC naming was a difficult process, no chemist would bother using it. You will soon realise that the naming process is very intuitive and almost seamless when practiced enough.

Rules for naming:

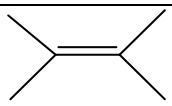
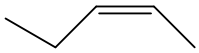
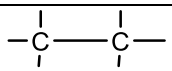
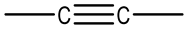
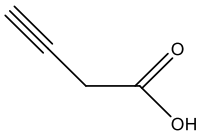
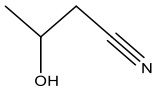
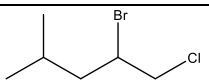
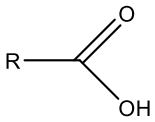
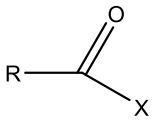
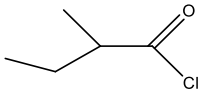
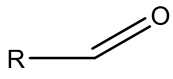
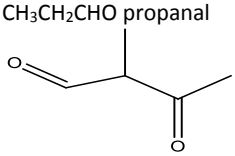
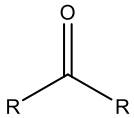
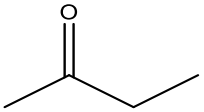
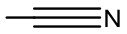
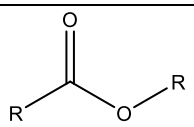
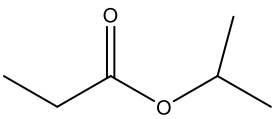
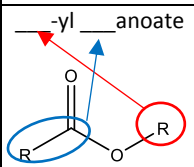
Before the rules of naming can be applied, a few terms must be remembered. These terms are the foundations of naming and everything else mentioned in this guide is just a build-up of that.

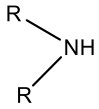
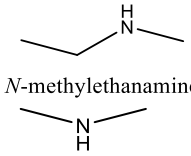
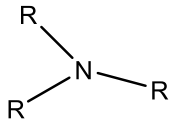
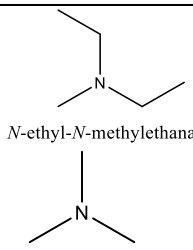
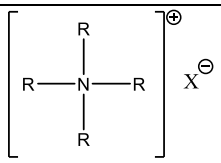
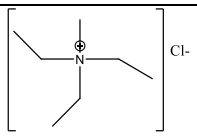
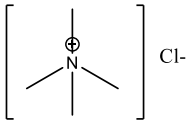
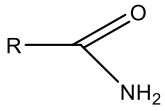
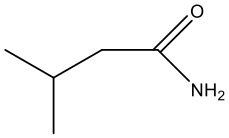
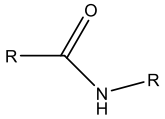
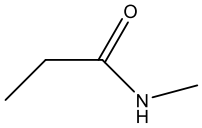
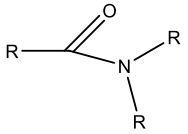
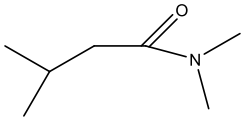
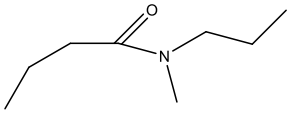
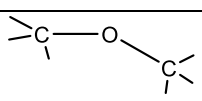
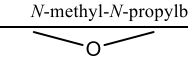
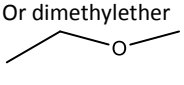
Code	Number of C atoms
Meth	1
Eth	2
Prop	3
But	4
Pent	5
Hex	6
Sept	7
Oct	8
Non	9
Dec	10

This allows us to identify the length of the parent chain or the size of any alkyl groups coming off the main parent chain.

Carboxylic acid
Ester
Acid halide
Amide
Nitrile
Aldehyde
Ketone
Alcohol
Amine
Ether
Alkane
Alkene
Alkyne
Halide
Nitro

Order of the priority of functional groups. For molecules with multiple groups, the group of higher priority takes the suffix of the name and is assigned a locant of 1. Other groups of lower priority take the prefix of the name.

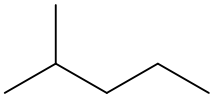
Functional group	Molecular formula	Prefix/ suffix	Example(s)	General name frame
Alkene		-ene [Note: may need to indicate if E/Z isomerism present]	CH_2=$CHCH_2CH_3$ but-1-ene  (*Z*)-pent-2-ene	
Alkane		-ane	$CH_3CH_2CH_3$ propane	
Alkyne		-yne/ -yn- alkenyl-	 but-2-yne  but-3-ynoic acid	
Alcohol	—OH	-ol hydroxy-	$CH_2OHCH_2CH_2OH$ propane-1,3-diol  3-hydroxybutanenitrile	
Haloalkane	C-X	chloro-, iodo-, bromo-, fluoro-	 2-bromo-1-chloro-4-methylpentane	
Carboxylic acid	 (-COOH)	-oic acid	CH_3COOH ethanoic acid $HOOCCH_2CH_2COOH$ butanedioic acid	__oic acid
Acyl halide	 -COX	-oyl halide [chloride, bromide etc]	CH_3COCl ethanoyl chloride  2-methylbutanoyl chloride	___-oyl halide
Aldehyde	 -CHO	-al formyl-	CH_3CH_2CHO propanal  2-methyl-3-oxobutanal	
Ketone	 -CO-	-one oxo- (in some cases you must use locants and in others you won't. Butan-2-one doesn't really need a 2 since the carbonyl group can only go in one position for it to be a ketone)	 butan-2-one	
Nitrile	 -CN	-nitrile cyano-	$CH_3CH_2CH_2CN$ butanenitrile	
Esters	 -COO-		$CH_3CH_2COOCH_3$ methyl propanoate  Propan-2-yl propanoate	___-yl ___anoate 
Primary amine	R—NH_2	-amine amino-	$CH_3CH_2NH_2$ ethylamine	___ylamine

Secondary amine			 *N*-methylethanamine dimethylamine	N-__yl(longest chain)-amine
Tertiary amine			 *N*-ethyl-*N*-methylethanamine trimethylamine	N-___ N-___ (longest chain)-amine alphabetically
Quaternary ammonium salt			 N, N-diethyl-N-methylammonium chloride  Tetramethylammonium chloride	N-__-N-___-N-___ ___ammonium [anion]
Primary amide		-amide	$CH_3CH_2CONH_2$ propanamide  3-methylbutanamide	
Secondary amide			 N-methyl propanamide	N-___yl ___amide
Tertiary amide			 *N*,*N*,3-trimethylbutanamide  *N*-methyl-*N*-propylbutyramide	N-___-N-___ ___amide Alphabetically
Ether		-ether alkoxy-	 methoxymethane Or dimethylether  methoxyethane	___oxy___ Longest chain

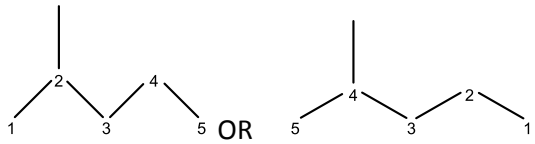
Most naming comes from identifying the parent chain and all the associated groups attached to it. It is then a case of simply deciding on the appropriate prefixes and suffixes to use to form the overall name. However, there may be situations where 'locants' and 'alphabetical order' must be used.

Locant:

With longer parent chains, we need to say where a side chain or functional group is located on the parent chain. This is done using a locant (number) in the name to tell us which C atom in the parent chain the group is attached to. The explanation of locant use will be shown using examples.

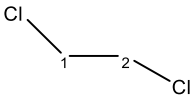


Here we have methylpentane (longest chain=5 C= -pent-, family=alkane= -ane, methyl group, CH_3 present so methyl-). We must make the position of the methyl group clear using locants, so we number the main carbon chain and see which number the methyl group is connected to.



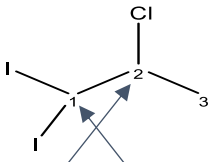
Notice how we could have started counting in either direction. Generally, we count in the direction that gives the smallest locant possible (unless another priority group defines the direction of counting). So, in this case, a locant of 2 is smaller than a locant of 4 so we use a locant of 2.

The name would therefore be 2-methylpentane. Locants are separated from words using hyphens (-).



Here we have 1,2-dichloroethane. Notice how we must use 2 locants to indicate the positions of both chlorine atoms (1 locant for each group). In this case the order of numbering doesn't matter since its 1,2 in either direction. When we use multiple locants, the direction of counting is chosen such that the sum of all the locants is as small as possible.

Strings of numbers are separated using commas (,).



2-chloro-1,1-diiodopropane.

Here we counted from the left to the right since locants of 1,1 and 2 give a smaller sum than 2,3,3 if we were to count from right to left.

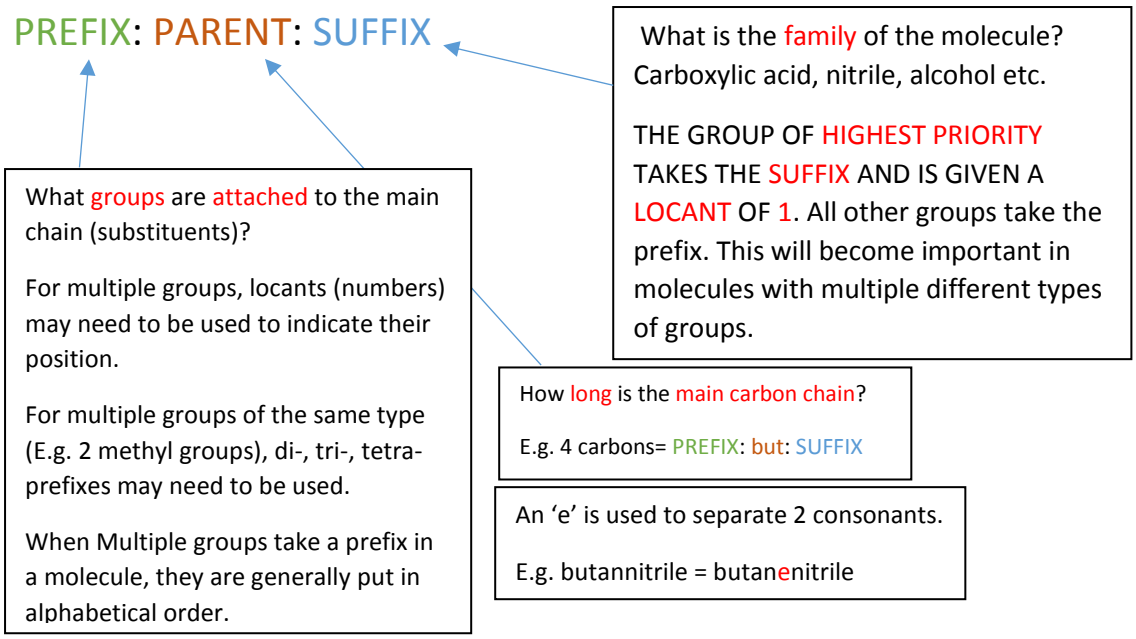
Chloro is written before iodo because we write the groups in alphabetical order. Notice how we ignore locants and di-, we only focus on the actual group name.

Alphabetical order example

General method for naming molecules:

1. Identify the longest carbon chain and decide the parent name (meth, eth, prop etc.).
2. Identify all functional groups present and determine the order of priority.
3. Use locants if necessary by numbering the main carbon chain.
4. If there are multiple substituents of the same functional group, use the appropriate prefix (di, tri. tetra etc.) to show the total number of them. Remember each group will still have its own locant.
5. Determine the appropriate prefixes, suffixes and the alphabetical order of groups. Using this, put together the name. Notice that there may be equivalent names which still refer to the same molecule (however, one will usually be preferred but both will still be correct).
6. To check the name, try and deduce the structure of the molecule using the name created.

The general name frame of a molecule can be written as follows:



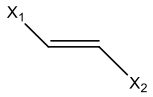
Other aspects of naming

E-Z (cis-trans) stereoisomerism:

These are to do with C=C bonds and arise due to restricted rotation about the C=C bond. E-Z isomerism only arises when there are 2 different groups/atoms attached to both ends of the C=C bond other than H.

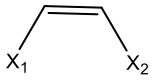
E isomerism:

E (or trans) isomerism: When the 2 groups are on opposite sides to each other.



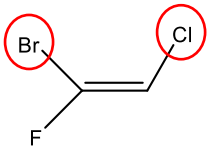
Z isomerism:

Z (or cis) isomers arise when there are 2 groups on the same side of the C=C bond.

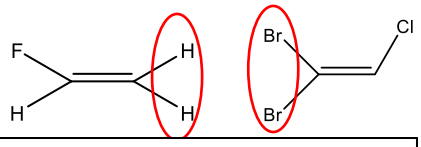


For alkenes with more than 2 groups around the double bond. The groups on either side of highest Mr/Ar are considered the priority groups that define whether its E or Z isomerism.

E.g.



On the left side, the highest Ar group is Br. On the right side the highest group is Cl. Therefore, Z



When we have groups of the same Mr/Ar like this around the double bond we DON'T have E/Z isomerism.

Naming: E/Z- (name of molecule). The molecule is named using the usual rules.

Z-1-bromo-2-chloro-1-floroethene for the example above.

Naming benzene based compounds:

http://www.chemguide.co.uk/basicorg/conventions/names3.html

If you require a more fundamental explanation of IUPAC naming, please refer to this website:

http://www.chem.uiuc.edu/GenChemReferences/nomenclature_rules.html