

Organic Nomenclature for the NSW HSC RACI NSW Chemical Education Group

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This RACI nomenclature document is being reissued due to growing concerns that teachers of chemistry are not using these rules correctly. In particular, the rules regarding haloalkane nomenclature need to be closely studied by all chemistry teachers as some textbooks and resources have not followed these rules. IUPAC uses the alphanumeric nomenclature system. Older methods using electronegativity differences between substituent groups are no longer valid.

Syllabus References	Relevant Stage 6 Chemistry Syllabus Content
<i>Preliminary Course</i>	
<ul style="list-style-type: none"> The Chemical Earth 8.2.1.2.8 Energy 8.5.2.2.3 8.5.3.2.2 	<ul style="list-style-type: none"> identify IUPAC names for carbon compounds as they are encountered identify that carbon can form single, double or triple covalent bonds with other carbon atoms identify and use the IUPAC nomenclature for describing straight-chained alkanes and alkenes from C1 to C8
<i>HSC Course</i>	
<ul style="list-style-type: none"> Production of Materials 9.2.3.2.9 The Acidic Environment 9.3.5.2.2 Chemical Monitoring and Management 9.4.4.2.9 	<ul style="list-style-type: none"> identify the IUPAC nomenclature for straight-chained alkanols from C1 to C8 identify the IUPAC nomenclature for describing the esters produced by reactions of straight-chained alkanolic acids from C1 to C8 and straight-chained primary alkanols from C1 to C8 identify and name examples of isomers (excluding geometrical and optical) of haloalkanes up to eight carbon atoms

Introduction

From the NSW Stage 6 Chemistry syllabus, students only need to name alkanes, alkenes, alkanols, esters and haloalkanes, although they may need to identify IUPAC names for other carbon compounds. While not completely explicit, it would seem a reasonable expectation that students can also name alkanolic acids, so they can reasonably name esters and write word equations for esterification.

The reference to straight-chained carbon compounds means students only need to name unbranched compounds, so there is no explicit requirement in the Preliminary Course to name compounds with carbon chain (alkyl) substituents. However, in the HSC Course students are required to name isomers of haloalkanes, which does not seem to exclude alkyl substituent chains as a possibility. The syllabus requires students to be aware of alkynes but does not explicitly require them to name them. The syllabus does not seem to exclude the possibility of multiple double bonds or hydroxyl groups with the naming of alkenes and alkanols.

Stems and functional groups

Before students can name any carbon compound, it is necessary for them to recognise and recall both the stems relating to the number of carbon atoms in an unbranched chain and any functional group that is in the compound. Carbon chains have little chemical function and so alkyl groups can be substituents but are not regarded as functional groups.

Below is a list of stems and functional groups. It is **NOT** necessary for students to name compounds with two or more **different** principal functional groups (eg a double bond AND an alcohol group) [see Appendix A for information for additional teacher interest only].

Number of C atoms and Carbon name stem	
1 meth –	5 pent –
2 eth –	6 hex –
3 prop –	7 hept –
4 but –	8 oct –

Family	Special feature	Suffix	Examples	Preferred IUPAC nomenclature*
Alkanes	C-C bonds	-ane	CH ₃ CH ₃ CH ₃ CH ₂ CH ₂ CH ₃	ethane butane
Alkenes	C=C bond (functional group)	-ene	CH ₂ CH ₂ CH ₂ CHCH ₂ CH ₃ CH ₃ CHCHCH ₃	ethylene but-1-ene but-2-ene
Alkanols	-OH (functional group)	-anol	CH ₃ CH ₂ OH CH ₃ CH ₂ CH ₂ OH CH ₃ CH(OH)CH ₃	ethanol propan-1-ol propan-2-ol
Alkanoic acids	-COOH (functional group)	-anoic acid	HCOOH CH ₃ COOH CH ₃ CH ₂ CH ₂ COOH	formic acid acetic acid butanoic acid
Esters	-COO- (functional group)	-anoate (formate, acetate)	HCOOCH ₃ CH ₃ COOC ₂ H ₅ CH ₃ CH ₂ COOCH ₃	methyl formate ethyl acetate methyl propanoate

(* Preferred IUPAC nomenclature is the most current and widely recognised system of chemistry nomenclature, particularly for naming organic molecules.

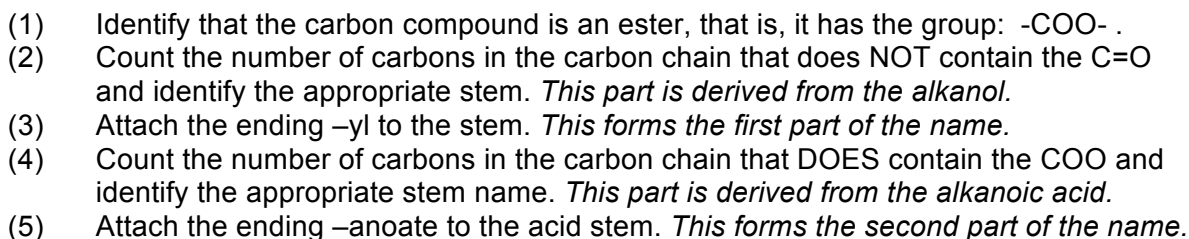
In a small number of cases, especially for commonly used substances, the IUPAC rules prefer use of so-called trivial names (eg ethylene, formic acid, acetic acid) over the equivalent, more systematic names (eg ethene, methanoic acid, ethanoic acid).

The following provides summary notes for naming particular HSC relevant classes of compounds. In each case the numbered steps shown should be followed in order. **Stop as soon as an unambiguous answer is obtained.**

- (1) Count the number of carbons in the longest unbranched chain and identify the appropriate carbon name stem.
- (2) Identify whether the carbon compound is an alkane, alkene, alkanol or alkanoic acid and add the appropriate suffix ending to the stem from the table above.
- (3) Number the chain from the end that produces the lowest set of locants (numbered positions) for the functional groups and substituents.
For alkenes, the locant is the number of the first carbon atom only of the two carbons of the alkene. Eg in ${}^1\text{CH}_3\text{-}^2\text{CH}=\text{}^3\text{CH-}^4\text{CH}_2\text{-}^5\text{CH}_3$ the locant for the alkene group is "2".
- (4) The numbers identifying the functional group are placed directly before the functional group portion of the name. The locant number is separated from other parts of the name by a hyphen.
The locant number is joined by hyphens to the carbon stem name and the suffix, when the functional group is indicated by a suffix, as in alkenes.

- When there is only one type of functional group and it is indicated as a suffix, the locant can be placed at the start of the systematic name as an alternative.
- No numbering is required for the alkanolic acids as it is assumed that the acid functional group is on carbon number 1.

(1) CH₃-CH₂-CH₂-CH=CH-CH₃ stem = hex
 suffix = ene
 locant = 2
Preferred IUPAC name : hex-2-ene
Alternative acceptable systematic name : 2-hexene



- (6) The complete name of the ester is then a combination of the alcohol and the acid names, listed in that order, as separate words.

Examples

- (1) $\text{CH}_3\text{CH}_2\text{COOCH}_3$ Derived from a one carbon alcohol, methyl, and three carbon acid, propanoate, so the correct name is methyl propanoate.
- (2) $\text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ Derived from a four carbon alcohol, butyl, and two carbon acid, ethanoate or acetate, so the preferred IUPAC name is butyl acetate.

3. Naming haloalkanes

Reminder, the following steps must be carried out in the order given:

- (1) Identify that the carbon compound contains halogens, that is, fluorine (F), chlorine (Cl), bromine (Br) and/or iodine (I). The halogen functional groups are named using prefixes placed in front of the name of the alkane, in alphabetical order:

Br: bromo- ; Cl: chloro- ; F: fluoro- ; I: iodo-

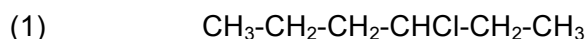
If there are more than one of any of the halogens, then the prefix di-, tri-, tetra-, etc is placed in front of the halogen name (eg 'difluoro' for two fluorine atoms).

- (2) Count the number of carbons in the longest unbranched carbon chain containing the halogen(s) and identify the appropriate stem name. Attach the -ane ending to the stem.
- (3) After identifying the longest chain, if there are any carbon substituent chains, count the number of carbons in each substituent chain, identify the appropriate stems and attach the -yl ending to them. If there are more than one of any of the carbon (now alkyl) substituent chains, then the prefix di-, tri-, tetra-, etc is placed in front of the alkyl substituent chain name (eg 'diethyl' for two two carbon substituent chains).
- (4) Assemble the components into a complete name, with the halogen and side group names placed in front of the main stem name, in alphabetical order, ignoring any di-, tri-, tetra-, etc prefixes. Eg 'dibromo' comes before 'chloro', see Examples (2) and (3).
- (5) Number the longest chain from the end that produces the lowest set of locants for all the halogen functional groups and alkyl substituents, and place locant number(s) in front of the respective halogen or substituent name, separated by a hyphen, and, where necessary, joined by a hyphen(s) to any earlier substituent name.
- NB:** When there is more than one halogen, the lowest set of locants is the set that, when compared term by term with other locant sets, **each cited in order of increasing value**, has the lowest term at the first point of difference.
- (6) If the previous rules lead to more than one possible name, then the correct name is the one in which **the lowest locant is assigned to the functional group cited first as a prefix**.

Notes:

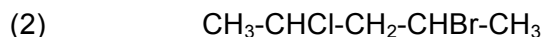
- (a) Each halogen and each alkyl group has its own number, even if on the same carbon atom,
eg 1,2-dichloroethane, 1,1-dichloroethane (NOT 1-dichloroethane),
2,2-dibromo-1-chloropropane, 1,3-dibromo-2-chloropropane, 1-bromo-2-methylpropane, 1,3-dibromo-2-methylbutane,
3-ethyl-4-fluorohexane, 4-ethyl-2-fluorohexane, 3-ethyl-5-fluoroheptane.

Examples:



The chain will be numbered from the right hand end as this will give the "chloro" group a locant of 3 on the chain rather than a locant of 4 if numbered from the left (Step 5).

The name of the molecule is: **3-chlorohexane**.



The molecule has five carbons in its longest unbranched chain (stem: "pent") and two different halogens, namely chlorine and bromine. To give a unique name to this molecule, place the halogen prefixes, in alphabetical order, before the stem name, then insert the locants. In this case, numbering from left or right gives the same minimum locant numbers (Step 5), but we apply the last Step (6) to give the prefix cited first the lowest locant (ie, bromine). Thus the chain is numbered from the left, and the "bromo" is at locant 2 and "chloro" is at locant 4.

The name of the molecule is: **2-bromo-4-chloropentane**

Q. What would be the correct name if the carbon chain was extended by one carbon to the right as written?

(7) *A. The correct IUPAC name for $\text{CH}_3\text{-CHCl-CH}_2\text{-CHBr-CH}_2\text{CH}_3$ is: **4-bromo-2-chlorohexane**, because numbering in this case must take place from the left to give the lowest set of locants (2 and 4 rather than 3 and 5, Step 5).*



The molecule contains a three carbon chain (stem: prop), and three halogen atoms, two chlorine (dichloro) and one fluorine (fluoro). We must assemble the halogen prefixes to the stem in the order: "dichloro" then "fluoro" because "c" comes before "f" in the alphabet (Step 4). Numbering from the right would give the name 2,3-dichloro-1-fluoropropane while numbering from the left would give the name 1,2-dichloro-3-fluoropropane. When we apply Step 5, we find the second name gives the first mentioned halogen(s) the lower set of locants, "1,2-dichloro" compared with the first, "2,3-dichloro". Thus the chain is numbered from the left.

The name of the molecule is: **1,2-dichloro-3-fluoropropane**



This molecule has only two carbons (stem: eth) and two halogens, chlorine and fluorine, with three of each halogen ("trichloro" and "trifluoro"). Following Steps 4 and then 5, numbering from the left end, the molecule would be named:

1,2,2-trichloro-1,1,2-trifluoroethane.

Numbering from the right end, the molecule would be named:

1,1,2-trichloro-1,2,2-trifluoroethane.

Thus the set of locants seem to be the same from either end, but they appear in different order.

Applying Step 6 allows us to give the molecule a unique name. Preference for the lowest locant set to the first named "chloro", rather than "fluoro".. That is, number the molecule from the right end.

The name of the molecule is: **1,1,2-trichloro-1,2,2-trifluoroethane**

Examples of IUPAC names converted into structures:

It is important that compounds are given names that are unambiguous, that is, names that lead to only one structure.

As a slightly more challenging exercise, and if you have not done so already, draw structures for each of the IUPAC names that appear in Note (a) on page 4, under Naming of haloalkanes.

In order to complete this task, work through the following steps, in order:

- (1) Identify the stem name and draw its structure. Eg "ethane", draw $\text{CH}_3\text{-CH}_3$.*
- (2) Identify the types of functional groups or substituents. Eg "Cl".*
- (3) Identify the number of each type of functional group or substituent. Eg "two".*
- (4) Use the locant numbers to identify the positions of the functional groups and substituents on the stem. Eg "positions 1- and 2-".*
- (5) Place the functional groups and substituents in their appropriate places on the stem, replacing or removing relevant hydrogen atoms as you go. Eg In steps " $\text{CH}_2\text{Cl-CH}_3$ then $\text{CH}_2\text{Cl-CH}_2\text{Cl}$ ".*
- (6) Check that the all atoms are accounted for and the molecular formula is complete. Eg All alkane carbons have four H or other atoms or groups attached to them.*

Answers:

1,2-dichloroethane, **$\text{CH}_2\text{Cl-CH}_2\text{Cl}$** | These two compounds have the same molecular
1,1-dichloroethane, **$\text{CHCl}_2\text{-CH}_3$** | formula, $\text{C}_2\text{H}_4\text{Cl}_2$, and so are ISOMERS of each
| other.

2,2-dibromo-1-chloropropane, **$\text{CH}_2\text{Cl-CBr}_2\text{-CH}_3$** | Notice that these two also have
1,3-dibromo-2-chloropropane, **$\text{CH}_2\text{Br-CHCl-CH}_2\text{Br}$** | the same formula, so are ISOMERS.

1-bromo-2-methylpropane, **$\text{CH}_2\text{Br-CHCH}_3\text{-CH}_3$**

Compare this with its unbranched chain isomer, 2-bromobutane, $\text{CH}_3\text{-CHBr-CH}_2\text{-CH}_3$. Both have the same molecular formulae, namely $\text{C}_4\text{H}_9\text{Br}$. How many unique unbranched isomers of bromobutane are there? (**A. Two.** They are: 1-bromobutane and 2-bromobutane. Note that 3-bromobutane and 4-bromobutane would be incorrect names.)

1,3-dibromo-2-methylbutane, **$\text{CH}_2\text{Br-CHCH}_3\text{-CHBr-CH}_3$**

3-ethyl-4-fluorohexane, **$\text{CH}_3\text{-CH}_2\text{-CHCH}_2\text{CH}_3\text{-CHF-CH}_2\text{-CH}_3$** | Same molecular formula,
4-ethyl-2-fluorohexane, **$\text{CH}_3\text{-CH}_2\text{-CHCH}_2\text{CH}_3\text{-CH}_2\text{-CHF-CH}_3$** | so they are ISOMERS.

3-ethyl-5-fluoroheptane, **$\text{CH}_3\text{-CH}_2\text{-CHCH}_2\text{CH}_3\text{-CH}_2\text{-CHF-CH}_2\text{-CH}_3$**

THE END

Appendix A - Additional Teacher Information

References

How about putting the 3 URLs for IUPAC in case teachers want to go back to original sources? This would seem more likely than referring them to the Journal article which is not necessary for HSC?

The International Union of Pure and Applied Chemistry (IUPAC) Blue Book (published in 1979 and revised in 1993) provides a helpful primary source of information. It comprises the accepted "Rules" from which these summary notes are derived:

Substitutive nomenclature – numbering

http://www.acdlabs.com/iupac/nomenclature/79/r79_883.htm

Halogen derivatives

http://www.acdlabs.com/iupac/nomenclature/79/r79_727.htm

Recommendation from 1993: 5.3.1

(see the second example for an illustration of the situation that has led to concerns in past HSC Chemistry paper on Haloalkane nomenclature.)

http://www.acdlabs.com/iupac/nomenclature/93/r93_370.htm

See also Journal of Chemical Education Vol. 83 No. 11 November 2006 pp1633-1637 (article *The IUPAC Rules for Naming Organic Molecules* by Stanislaw Skonieczny).

The university libraries mostly will subscribe to this journal. If your school library also subscribes to the Journal, it can be accessed at <http://www.JCE.DivCHED.org>

This article discusses nomenclature where there are more than two different principal groups. It contains a table of Order of Precedence for the Major Functional Groups. It concerns the naming of very complex structures with sulfur and nitrogen substitutions as well as benzene ring derivatives and cycloalkanes.

It contains these extra points **not necessary** for HSC chemistry:

- (a) If the principal functional group occurs in a chain, the principal chain is selected as
 - (i) the chain containing the functional group of the highest order of precedence.
(*Eg, an OH group is higher than a halide group, so a compound would be named, say, 2-chlorohexan-2-ol not 2-chloro-2-hydroxyhexane.*
Eg, the ketone group is higher than the -OH group, so a compound would be named, for example, as 4-hydroxypentan-2-one rather than 4-oxopentan-2-ol.
Eg, compounds with both double and triple bonds are called enynes and the triple bond has precedence over the double bond regarding numbering. Thus, hept-5-en-2-yne is the preferred systematic name for the molecule that has a triple bond from carbons 2 to 3 and a double bond from carbon atoms 5 to 6.)
 - (ii) If more than one such choice is possible, select the chain with the maximum number of double bonds.
 - (iii) If points (i) and (ii) together are not definitive, then choose the chain with the maximum length.
 - (iv) If two chains of the same length are possible, choose the one with the maximum number of substituents.
- (b) If the principal functional group occurs in a cyclic system, that system forms the parent.