GRADE 12 PHYSICAL SCIENCES

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IUPAC naming and formulae 4.3

What is IUPAC naming?

In order to give compounds a name, certain rules must be followed. When naming organic compounds, the IUPAC (International Union of Pure and Applied Chemistry) nomenclature (naming scheme) is used. This is to give consistency to the names. It also enables every compound to have a unique name, which is not possible with the common names used (for example in industry). We will first look at some of the steps that need to be followed when naming a compound, and then try to apply these rules to some specific examples.

A good general rule to follow is to start at the end (the suffix) and work backwards (from right to left) in the name.

- 1. Recognise the *functional group* in the compound. This will determine the suffix of the name (see Table 4.5).
- 2. Find the longest continuous carbon chain that contains the functional group (it won't always be a straight chain) and count the number of carbon atoms in this chain.

This number will determine the pre-fix (the beginning) of the compound's name (see Table 4.6).

- 3. Number the carbons in the longest carbon chain (Important: If the molecule is not an alkane (i.e. has a functional group) you need to start numbering so that the *functional group* is on the carbon with the lowest possi-ble number). Start with the carbon at the end closest to the functional group.
- 4. Look for any branched groups:
 - Name them by counting the number of carbon atoms in the branched group and referring to Table 4.6, these groups will all end in -yl.
 - Note the position of the group on the main carbon chain. If there is more than one of the same type of branched group then both numbers must be listed (e.g. 2,4 -) and one of the prefixes listed in Table 4.7 must be used. **Important:** If the molecule is an *alkane* the branched group must be on the carbon with the lowest possible number.
 - The branched groups must be listed before the name of the main chain in alphabetical order (ignoring di/tri/tetra). If there are no branched groups this step can be ignored.

Number	prefix
2	di-
3	tri-
4	tetra-

Table 4.7: Prefixes for multiple substituents with the same name. These apply to multiple functional groups as well.

- 5. For the alkyl halides the halogen atom is treated in much the same way as branched groups:
 - To name them take the name of the halogen atom (e.g. iodine) and replace the -ine with -o (e.g. iodo).

suffix
-ane
-ene
-yne
-ol
-al
-one
-oic acid
-oate

Table 4.5:The suffix associated with various functional groups.

Carbon atoms	prefix	
1	meth-	
2	eth-	
3	prop-	
4	but-	
5	pent-	
6	hex-	
7	hept-	
8	oct-	
9	non-	
10	dec-	

TIP

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Molecules can contain both double or triple bonds and other functional groups (e.g. an alkene and an alcohol functional group in one molecule - propenol). However, all molecules explored in this book will contain only single carbon-carbon bonds when combined with other functional groups.

Table 4.6: The prefix of a compound's name is determined by he number of carbon atoms in he longest chain hat contains the unctional group.

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- Give the halogen atom a number to show its position on the carbon chain. If there is more than one halogen atom the numbers should be listed and a prefix should be used (e.g. 3,4-diiodo- or 1,2,2-trichloro-). See Table 4.7 for a list of the prefixes.
- The halogen atoms must be listed before the name of the main chain in alphabetical order (ignore di/tri/ tetra).
- If there are no halogen atoms this step can be ignored.
- 6. Combine the elements of the name into a single word in the following order:
 - branched groups/halogen atoms in alphabetical order (ignoring prefixes)
 - prefix of main chain
 - name ending according to the functional group and its position on the longest carbon chain.

Naming hydrocarbons

Naming alkanes

The suffix for an alkane is -ane.

Worked example 1: Naming the alkanes

QUESTION н н н н Give the IUPAC name for the following compound: — C(4) - $-C_{(1)} - C_{(2)} - C_{(3)} -$ - H Note: The numbers attached to the Ĥ Ĥ Ĥ Ĥ carbon atoms would not normally be

The carbon atoms have been numbered to help you to name the compound.

SOLUTION

shown.

Step 1: Identify the functional group

The compound is a hydrocarbon with single bonds between the carbon atoms. It is an alkane and will have a suffix of -ane.

Step 2: Find the longest carbon chain

There are four carbon atoms in the longest chain. The prefix of the compound will be but-.

Step 3: Number the carbon atoms in the longest chain

The numbering has been done for you here.

Step 4: Look for any branched group, name them and give their position on the carbon chain

There are no branched groups in this compound.

Halogen	name
fluorine	fluoro
chlorine	chloro
bromine	bromo
iodine	iodo

Table 4.8: Naming halogen atoms in organic molecules.

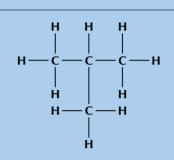
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Step 5: Combine the elements of the name into a single word The name of the compound is **butane**.

Worked example 2: Naming the alkanes

QUESTION

Give the IUPAC name for the following compound:



SOLUTION

Step 1: Identify the functional group

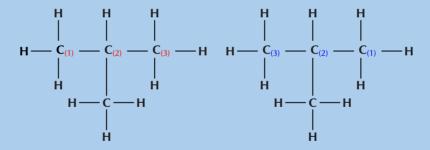
The compound is a hydrocarbon with single bonds between the carbon atoms. It is an alkane and will have the suffix -ane.

Step 2: Find the longest carbon chain

There are three carbon atoms in the longest chain. The prefix for this compound is prop-.

Step 3: Number the carbons in the carbon chain

If we start at the carbon on the left, we can number the atoms as shown in red (left). If we start at the carbon on the right, we can number the atoms as shown in blue (right).



Step 4: Look for any branched groups, name them and give their position on the carbon chain

There is a branched group attached to the second carbon atom. In this case the methyl group is on carbon 2 regardless of which side you number the longest chain from.

This group has the formula CH_3 , which is methane without a hydrogen atom. However, because it is not part of the main chain, it is given the suffix -yl (i.e. methyl). The position of the methyl group comes just before its name (see the next step).

Step 5: Combine the elements of the compound's name into a single word in the order of branched group; prefix; name ending according to the functional group The compound's name is **2-methylpropane**.

Worked example 3: Naming the alkanes

QUESTION

Draw the semi-structural structural and condensed structural formula for the organic compound **2,2,4-trimethylhexane**

SOLUTION

Step 1: Identify the functional group

The name ends in -ane therefore the compound is an alkane.

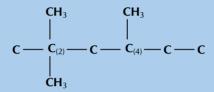
Step 2: Determine the number of carbon atoms in the longest chain

The longest chain has the prefix hex-. There are therefore 6 carbon atoms in the longest chain.

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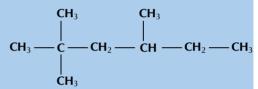
Step 3: Look for any branched groups and place them on the structure

The compound is **2,2,4-trimethyl**hexane. Therefore there are three branched groups. Two on carbon 2 and one on carbon 4.



Step 4: Combine this information and add the hydrogen atoms

Carbon atoms can have four single bonds. Therefore wherever a carbon atom has less than four bonds draw in hydrogen atoms until there are four bonds.



Step 5: Condense the structural formula

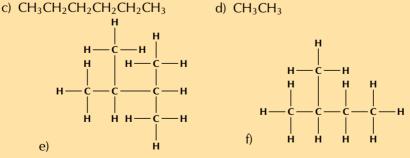
First condense the main chain: CH₃CCH₂CHCH₂CH₃

Then add the side chains (in brackets) on the relevant carbon atoms:

$\textbf{CH}_3\textbf{C}(\textbf{CH}_3)_2\textbf{CH}_2\textbf{CH}(\textbf{CH}_3)\textbf{CH}_2\textbf{CH}_3$

Exercise 4 – 8: Naming alkanes

- 1. Give the structural formula for each of the following alkanes
 - a) Octane b) Propane c) 2-methylpropane d) 3-ethylpentane
- 2. Give the IUPAC name for each of the following alkanes:
 - a) CH₃CH₂CH(CH₃)CH₂CH₃ b) CH₃CH(CH₃)CH₂CH(CH₃)CH₃



3. More questions. Sign in at Everything Science online and click 'Practise Science'. Check answers online with the exercise code below or click on 'show me the answer'.

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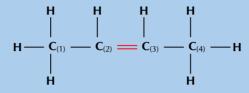
Naming alkenes

The suffix for an alkene is -ene.

Worked example 4: Naming the alkenes

QUESTION

Give the IUPAC name for the following compound:



SOLUTION

Step 1: Identify the functional group

The compound has a double carbon-carbon bond and is an alkene. It will have the suffix -ene.

Step 2: Find the longest carbon chain containing the functional group

The functional group is a double bond, so the longest chain must contain the double bond. There are four carbon atoms in the longest chain and so the prefix for this compound will be but-.

Step 3: Number the carbon atoms

Remember that the carbon atoms must be numbered so that the functional group is at the lowest numbered carbon atom possible. In this case, it doesn't matter whether we number the carbons from the left to right, or from the right to left. The double bond will still fall between the second and third carbon atoms.

Step 4: Look for any branched groups, name them and give their position on the carbon chain

There are no branched groups in this molecule.

Step 5: Combine the elements of the name into a single word in the following order: branched groups; prefix; name ending according to the functional group and its position along the longest carbon chain

The name of this compound is **but-2-ene** or **2-butene**.

Worked example 5: Naming the alkenes

QUESTION

Draw the structural and molecular formula for the organic compound **3-methylbut-1-ene**

SOLUTION

Step 1: Identify the functional group

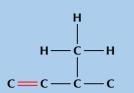
The suffix -ene means that this compound is an alkene and there must be a double bond in the molecule. The number 1 immediately before the suffix means that the double bond must be at the first carbon in the chain (but-1-ene).

Step 2: Determine the number of carbon atoms in the longest chain containing the functional group

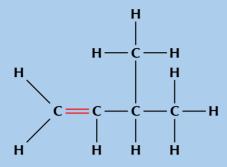
The prefix for the compound is but- so there must be four carbons in the longest chain containing the double bond. c = c - c - c

Step 3: Look for any branched groups

There is a methyl group at the third carbon atom in the chain. Count from the left so that the double bond carbon is the first carbon atom.

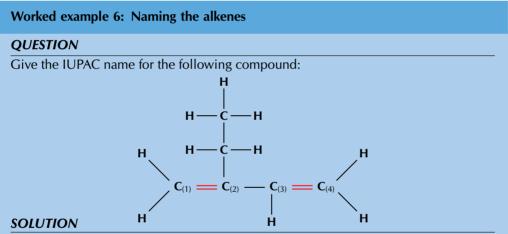


Step 4: Combine this information and add the hydrogen atoms



Step 5: Reduce the structural formula to the molecular formula

There are 5 carbon atoms and 10 hydrogen atoms so the molecular formula is C_5H_{10} . (Remember that there is no *structural* information given by the molecular formula)



Step 1: Identify the functional group

The compound is an alkene and will have the suffix -ene. There is a double bond between the first and second carbons and also between the third and fourth carbons. The organic compound therefore contains '1,3-diene'.

Step 2: Find the longest carbon chain containing the functional group, and number the carbon atoms

Remember that the main carbon chain must contain both the double bonds. There are four carbon atoms in the longest chain containing the double bonds and so the prefix for this compound will be but-. The carbon atoms are already numbered 1 to 4 in the diagram.

Step 3: Look for any branched groups, name them and give their position on the carbon chain

There is an ethyl group on the second carbon.

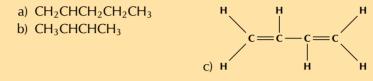
Note that if we had numbered from the right to left the suffix would still have been 1,3-diene, however the ethyl group would have been on the third carbon. So we had to number left to right.

Step 4: Combine the elements of the name into a single word in the following order: branched groups; prefix; name ending according to the functional group and its position along the longest carbon chain

The name of this compound is 2-ethylbut-1,3-diene.

Exercise 4 – 9: Naming alkenes

1. Give the IUPAC name for each of the following alkenes:



2. Give the structural formula for each of the following alkenes:

c) hept-3-ene d) 4-ethyloct-3-ene a) ethene b) hex-1-ene

3. More questions. Sign in at Everything Science online and click 'Practise Science'.

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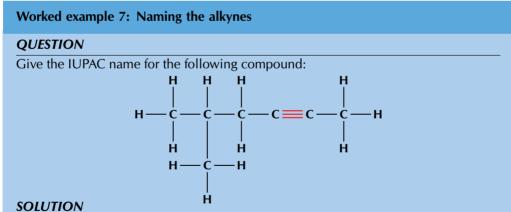
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Naming alkynes

The suffix for an alkyne is -yne.



Step 1: Identify the functional group

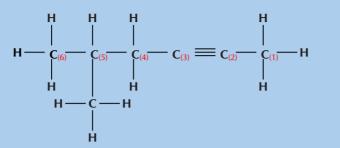
There is a triple bond between two of the carbon atoms, so this compound is an alkyne. The suffix will be -yne.

Step 2: Find the longest carbon chain containing the functional group

The functional group is a triple bond, so the longest chain must contain the triple bond. There are six carbon atoms in the longest chain. The prefix of the compound's name will be hex-.

Step 3: Number the carbons in the longest chain

In this example, you will need to number the carbons from right to left so that the triple bond is between carbon atoms with the lowest numbers (the suffix for the compound will therefore be -2-yne).



Step 4: Look for any branched groups, name them and assign the number of the carbon atom to which the group is attached

There is a methyl (CH_3) group attached to the fifth carbon (remember we have numbered the carbon atoms from right to left).

Step 5: Combine the elements of the name into a single word in the following order: branched groups; prefix; name ending according to the functional group and its position along the longest carbon chain

If we follow this order, the name of the compound is **5-methylhex-2-yne**.

Worked example 8: Naming the alkynes

OUESTION

Give the IUPAC name for the following compound:

$$\mathsf{CH} = \mathsf{C} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{C} = \mathsf{C} - \mathsf{CH}_3$$

SOLUTION

Step 1: Identify the functional group

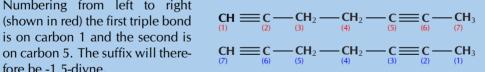
There are two triple bonds. The suffix will therefore be -diyne.

Step 2: Find the longest carbon chain containing the functional group

The functional group is a triple bond, so the longest chain must contain all triple bonds. The longest carbon chain contains seven carbon atoms, therefore the prefix will be hept-.

Step 3: Number the carbons in the longest chain

Numbering from left to right (shown in red) the first triple bond is on carbon 1 and the second is fore be -1,5-divne.



(Numbering from right to left (shown in blue) will give the suffix -2,6-diyne, and is incorrect).

Step 4: Look for any branched groups

There are no branched groups for this molecule.

Step 5: Combine the elements of the name into a single word in the following order: branched groups; prefix; name ending according to the functional group and its position along the longest carbon chain

The name of the compound is **hept-1,5-diyne**.

Worked example 9: Naming the alkynes

QUESTION

Draw the structural and condensed structural formula for the organic compound **6-methylhept-3-yne**

SOLUTION

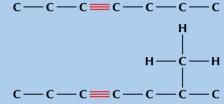
number 6.

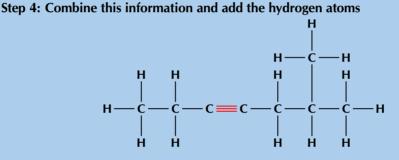
Step 1: Identify the functional group

The suffix -3-yne means that this compound is an alkyne and there must be a triple bond located on carbon number 3.

Step 2: Determine the number of carbon atoms in the longest chain containing the functional group

Step 3: Look for any branched groups There is a methyl group located on carbon



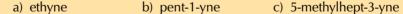


Step 5: Condense the structural formula

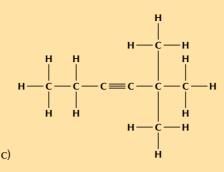
First condense the main chain: $CH_3CH_2CCCH_2CHCH_3$ Then add the side chains (in brackets) on the relevant carbon atoms: $CH_3CH_2CCCH_2CH(CH_3)CH_3$

Exercise 4 – 10: Naming alkynes

1. Give the structural formula for each of the following alkynes:



2. Give the IUPAC names for the following alkynes:



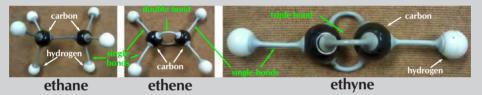
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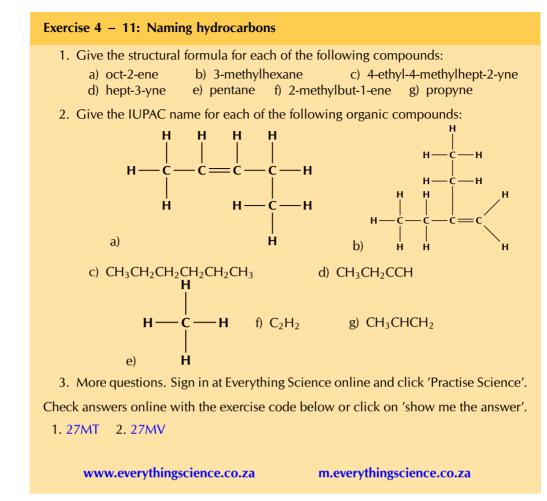
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Activity: Building hydrocarbons

An example of ethane, ethene and ethyne built with atomic model kits is given in the picture below:



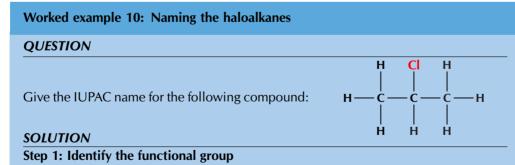
- 1. Using atomic model kits, build the molecules of methane, propane, butane, pentane and octane. If you don't have atomic model kits, jelly tots (or playdough) and toothpicks will work just as well. Use one colour jelly tot for the carbon atoms and one for the hydrogen atoms.
 - Remember that carbon atoms should have four bonds and hydrogen atoms can have only one. You should see that all these compounds have a similar formula, remember they all have the general formula C_nH_{2n+2} .
 - What is the name of the homologous series that all these molecules belong to?
- 2. Build the molecules of prop-1-ene, but-1-ene, pent-1-ene and oct-1-ene. Use two toothpicks to represent a double bond. You should see that all these compounds have a similar formula. Remember, they all have the general formula C_nH_{2n} .
 - Try placing the double bond at different positions within the molecule. Does this make any difference to the total number of carbon and hydrogen atoms in the molecule?
 - What is the name of the homologous series that all these molecules belong to?
- 3. Build the molecules of prop-1-yne, but-1-yne, pent-1-yne and oct-1-yne. Use three toothpicks to represent a triple bond. You should see that all these compounds have a similar formula. Remember, they are all alkynes.
 - Try placing the triple bond at different positions within the molecule. Does this make any difference to the total number of carbon and hydrogen atoms in the molecule?
 - What is the general formula for the alkynes?



Naming alkyl halides

All the same rules apply when naming the alkyl halides as for naming the hydrocarbons. We will only be dealing with the haloalkanes (i.e. there are no other functional groups). The halogen atom is treated in the same way as a branched group.

ESCKK



There is a halogen atom and no other functional group. This compound is therefore a haloalkane, and will have the suffix -ane.

Step 2: Find the longest carbon chain containing the functional group

There are three carbons in the longest chain containing the halogen atom. The prefix is prop-.

Step 3: Number the carbon atoms in the longest chain

You need to number the carbon atoms so that the halogen atom is on the carbon atom

with the lowest number. In this case you can number from either side.

Step 4: Name the halogen atom and assign the number for the carbon atom it is attached to

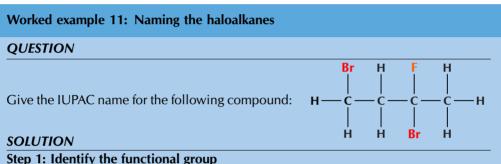
The halogen is a chlorine atom. It is attached to carbon number 2 and so will have the name 2-chloro.

Step 5: Look for branched groups

There are no branched groups in this compound.

Step 6: Combine the elements of the name into a single word in the following order: halogen atoms; prefix; name ending according to functional group

The name of the compound is 2-chloropropane.



There are three halogen atoms and no other functional groups. This compound is therefore a haloalkane, and will have the suffix -ane.

Step 2: Find the longest carbon chain containing the functional group

There are four carbons in the longest chain containing all the halogen atoms. The prefix for this compound will be but-.

Step 3: Number the carbon atoms in the longest chain

You need to number the carbon atoms so that the halogen atoms are on the carbon atoms with the lowest numbers. You must number from left to right here so that one halogen atom is on carbon 1 and two halogen atoms are on carbon 3.

Step 4: Name the halogen atoms and assign the number for the carbon atom attached to it

There are two halogen atoms that are bromine atoms and one that is fluorine. One bromine is attached to carbon 1 and one is attached to carbon 3. The fluorine atom is attached to carbon 3. So you have 1,3-dibromo- and 3-fluoro.

Step 5: Look for branched groups

There are no branched groups in this compound.

Step 6: Combine the elements of the name into a single word in the following order: halogen atoms in alphabetical order; prefix; name ending according to functional group

The name of the compound is **1,3-dibromo-3-fluorobutane**. Note that we place the halogens in alphabetical order: *b*romo (ignore the di/tri/tetra) is before *f*luoro.

Worked example 12: Naming the haloalkanes

QUESTION

Draw the structural and condensed structural formula for the organic compound **2-iodo-3-methylpentane**

SOLUTION

Step 1: Identify the functional group

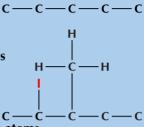
This compound has the suffix -ane, but also contains a halogen atom. It is therefore a haloalkane. Note that the methyl and iodo are written in alphabetical order.

Step 2: Find the longest carbon chain containing the functional group

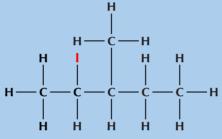
The prefix is pent- therefore there are 5 carbons in the longest chain.

Step 3: Place the halogen atom(s) and any branched groups

There is an iodine atom on the second carbon atom, and a methyl branched group on the third carbon atom.



Step 4: Combine this information to and add the hydrogen atoms



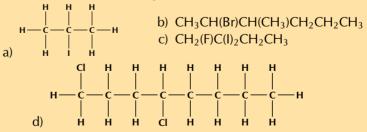
Step 5: Condense the structural formula

First condense the main chain: CH₃CHCHCH₂CH₃

Then add the side chains and halogen atoms (in brackets) on the relevant carbon atoms: $CH_3CH(I)CH(CH_3)CH_2CH_3$

Exercise 4 – 12: Naming haloalkanes

- 1. Give the structural representation for the following haloalkanes:
- a) 2-chlorobutane b) 1-bromopropane c) 2,3-difluoropentane
- 2. Give the IUPAC name for the following haloalkanes:



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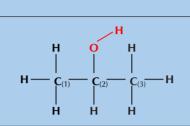
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The rules used to name the alcohols are similar to those already discussed for the hydrocarbons. The suffix of an alcohol is -ol (see Table 4.5).

Worked example 13: Naming the alcohols

OUESTION

Give the IUPAC name for the following organic compound



SOLUTION

Step 1: Identify the functional group

The compound has an -OH (hydroxyl) functional group and is therefore an alcohol. The compound will have the suffix -ol.

Step 2: Find the longest carbon chain containing the functional group

There are three carbon atoms in the longest chain that contains the functional group. The prefix for this compound will be prop. As there are only single bonds between the carbon atoms, the prefix includes an to become propan-.

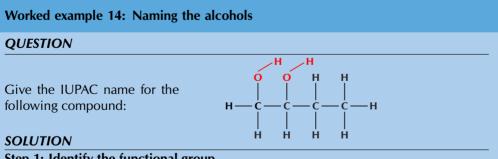
Step 3: Number the carbons in the carbon chain

In this case, it doesn't matter whether you start numbering from the left or right. The hydroxyl group will still be attached to second carbon atom (-2-ol).

Step 4: Look for branched groups

There are no branched groups in this compound.

Step 5: Combine the elements of the compound's name into a single word in the order of branched groups; prefix; name ending according to the functional group The compound's name is **propan-2-ol** or **2-propanol**.

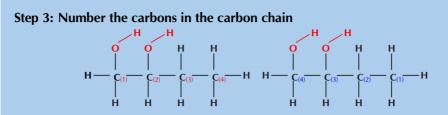


Step 1: Identify the functional group

The compound has an -OH (hydroxyl) functional group and is therefore an alcohol. There are two hydroxyl groups in the compound, so the suffix will be -diol.

Step 2: Find the longest carbon chain that contains the functional group

There are four carbon atoms in the longest chain that contains the functional group (but-) and only single bonds (an-). The prefix for this compound will be butan-.



There are two hydroxyl groups attached to the main chain. If we number as shown in red (on the left) they are attached to the first and second carbon atoms. If we number as shown in blue (on the right) they are attached to the third and fourth carbon atoms.

The functional groups should have the lowest numbers possible. Therefore the red numbering is correct. The hydroxyl groups are attached to the first and second carbon atoms (1,2-diol).

Step 4: Look for branched groups

There are no branched groups in this compound.

Step 5: Combine the elements of the compound's name into a single word in the order of branched groups; prefix; name ending according to the functional group The compound's name is **butan-1,2-diol**.

Worked example 15: Naming the alcohols

QUESTION

Draw the structural and condensed structural representations for the organic compound **4-ethyloctan-2,5-diol**

SOLUTION

Step 1: Identify the functional group

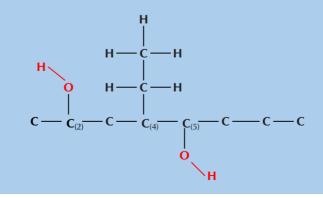
The compound has the suffix -ol. It is therefore an alcohol.

Step 2: Find the longest carbon chain that contains the functional group

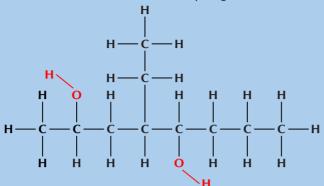
The prefix is oct- therefore there are 8 carbons in the longest chain containing the functional group. C - C - C - C - C - C - C - C

Step 3: Place the functional group as well as any branched groups

There is one -OH attached to carbon 2 and one attached to carbon 5. There is also an ethyl ($-CH_2CH_3$) branched group attached to carbon 4.



Step 4: Combine this information and add the hydrogen atoms



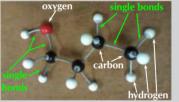
Step 5: Condense the structural formula

First condense the main chain: $CH_3CHCH_2CHCHCH_2CH_2CH_3$ Then add the side chains and alcohol functional groups (in brackets) on the relevant carbon atoms: $CH_3CH(OH)CH_2CH(CH_2CH_3)CH(OH)CH_2CH_2CH_3$

Activity: Building alcohols

The structural representation of butan-1-ol built using an atomic model kit is given below:

Using atomic model kits, build the molecules of methanol, ethanol, propan-1-ol, pentan-1-ol and octan-1-ol. If you don't have an atomic model kit remember that you can use jelly tots (or playdough) and toothpicks. Use different colour jelly tots to represent the different atoms.



butan-1-ol

 $-CH_2 - CH_2 - CH_3$

- You should see that all these compounds have a similar formula. Remember, they belong to the homologous series of the alcohols. What is the general formula for this series?
- Try placing the hydroxyl group at different positions within the molecule. Does this make any difference to the total number of carbon, hydrogen and oxygen atoms in the molecule?

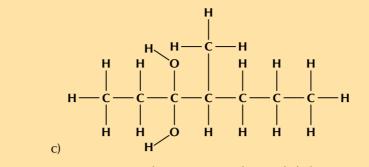
Exercise 4 – 13: Naming alcohols

- 1. Give the structural representation of each of the following organic compounds: a) pentan-3-ol b) butan-2,3-diol c) 2-methylpropan-1-ol
- 2. Give the IUPAC name for each of the following:
 - a) CH₃CH₂CH(OH)CH₃

ols. What is the general formula selfende ositions within the molecule. r of carbon, hydrogen and o

b)

ЮH



3. More questions. Sign in at Everything Science online and click 'Practise Science'. Check answers online with the exercise code below or click on 'show me the answer'.

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ESCKN

Naming carbonyl compounds

A carbonyl group consists of a carbon atom that is bonded to an oxygen atom through a double bond (C=O). There are many different functional groups that contain a carbonyl group.

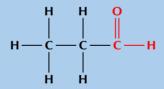
Naming aldehydes

If the carbonyl group is on the *end* of the carbon chain, the organic compound is called an *aldehyde*. An aldehyde has the suffix -al.

Worked example 16: Naming aldehydes

QUESTION

Give the IUPAC name and molecular formula for the following organic compound



SOLUTION

Step 1: Identify the functional group

The compound has a C=O (carbonyl) group and no other functional groups. It is therefore either an aldehyde or a ketone. The carbonyl group is on the last (terminal) carbon in the main chain so the compound is an aldehyde. It will have the suffix -al.

Step 2: Find the longest carbon chain containing the functional group

There are three carbons in the longest chain that contains the functional group. The prefix for this compound will be prop-. As there are only single bonds between the carbon atoms, the prefix becomes propan-.

Step 3: Number the carbon atoms in the carbon chain

The carbon atoms will be numbered so that the carbon atom of the aldehyde group has the lowest number possible. In this case that is from right to left.

Step 4: Look for any branched groups

There are no branched groups in this compound.

Step 5: Combine the elements of the compound's name into a single word in the order of branched groups; prefix; name ending according to the functional group

The compound's name is **propanal** (there is no need to say propan-1-al as by definition all aldehydes are -1-al).

Step 6: Reduce the structural representation to the molecular formula

There are 3 carbon atoms, 6 hydrogen atoms and 1 oxygen atom so the molecular formula is C_3H_6O .

(Remember that there is no structural information given by the molecular formula)

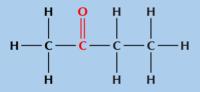
Naming ketones

If the carbonyl group is in the middle of the carbon chain, the compound is called a *ketone*. A ketone has the suffix -one.

Worked example 17: Naming ketones

QUESTION

Give the IUPAC name and molecular formula for the following compound:



SOLUTION

Step 1: Identify the functional group

The compound has a C=O (carbonyl) group and no other functional groups. It is therefore either an aldehyde or a ketone. The carbonyl group is **not** at the end of the chain. Therefore the compound is a ketone and the suffix will be -one.

Step 2: Find the longest carbon chain containing the functional group

There are four carbons in the longest chain that contains the functional group, and only single carbon-carbon bonds. The prefix for this compound will be butan.

Step 3: Number the carbon atoms in the carbon chain

The carbon atoms will be numbered from left to right so that the carbon atom of the ketone group has the lowest number possible (-2-one).

Step 4: Look for any branched groups

There are no branched groups in this compound.

Step 5: Combine the elements of the compound's name into a single word in the order of branched groups; prefix, name ending according to the functional group The compound's name is **butan-2-one** or **2-butanone**.

Step 6: Reduce the structural representation to the molecular formula

There are 4 carbon atoms, 8 hydrogen atoms and 1 oxygen atom so the molecular formula is C_4H_8O .

(Remember that there is no *structural* information given by the molecular formula)

TIP

Ketone is pronounced *key***tone**. Therefore propanone is pronounced propan**own**.

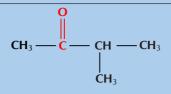
FACT

Note that butanone can only be butan-2-one. If the carbonyl group were on carbon 1 it would be an aldehyde, while if it were on carbon 3 we would simply count from the other side of the molecule. The 2 is still required for IUPAC naming however.

Worked example 18: Naming carbonyl compounds

QUESTION

Give the IUPAC name for the following compound:



SOLUTION

Step 1: Identify the functional group

The compound has a C=O (carbonyl) group and no other functional groups. It is therefore either an aldehyde or a ketone. The carbonyl group is **not** at the end of the chain. Therefore the compound is a ketone and the suffix will be -one.

Step 2: Find the longest carbon chain that contains the functional group

The longest carbon chain that contains the functional group has four carbon atoms in it, and only single bonds. The prefix for this compound will be butan-.

Step 3: Number the carbon atoms in the carbon chain

The carbon atoms will be numbered from left to right so that the carbon atom of the ketone functional group has the lowest possible number. The suffix will be -2-one.

Step 4: Look for any branched groups

There is a branched group on carbon 3. This group has only one carbon atom. The branched group is attached to the third carbon atom (3-methyl).

Step 5: Combine the elements of the compound's name into a single word in the order of branched groups; prefix; name ending according to the functional group The compound's name is **3-methylbutan-2-one**.

Worked example 19: Naming carbonyl compounds

QUESTION

Draw the structural and condensed structural representations for the organic compound **3-methylpentanal**.

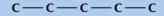
SOLUTION

Step 1: Identify the functional group

The compound has the suffix -al. It is therefore an aldehyde and has a C = O (carbonyl) group on the first carbon atom.

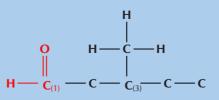
Step 2: Find the longest carbon chain that contains the functional group

The prefix is pent- so there are 5 carbon atoms in the longest chain.

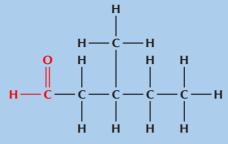


Step 3: Place the functional group as well as any branched groups

There is a C = O (carbonyl) group at the first carbon atom and a methyl group attached to the third carbon atom (3-methyl).



Step 4: Combine this information and add the hydrogen atoms



Step 5: Condense the structural representation

First condense the main chain including the carbonyl group oxygen atom: $CHOCH_2CHCH_2CH_3$

Then add the side chains on the relevant carbon atoms: CHOCH₂CH(CH₃)CH₂CH₃

Worked example 20: Naming carbonyl compounds

QUESTION

Draw the structural and condensed structural representations for the organic compound **3-methylpentan-2-one**.

SOLUTION

Step 1: Identify the functional group

The compound has the suffix -one. It is therefore a ketone and has a C=O (carbonyl) group. This group *cannot* be on the first carbon atom.

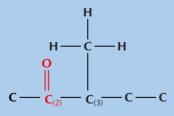
Step 2: Find the longest carbon chain that contains the functional group

The prefix is pent- therefore there are 5 carbon atoms in the longest chain.

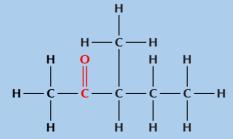
c—c—c—c—c

Step 3: Place the functional group as well as any branched groups

There is a C=O (carbonyl) group at the second carbon atom (-2-one) and a methyl group attached to the third carbon atom (3-methyl).



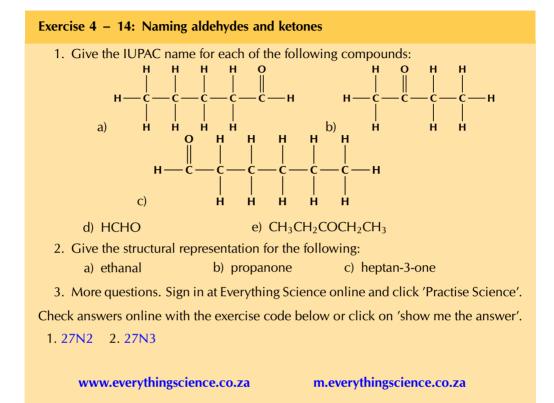
Step 4: Combine this information and add the hydrogen atoms



Step 5: Condense the structural representation

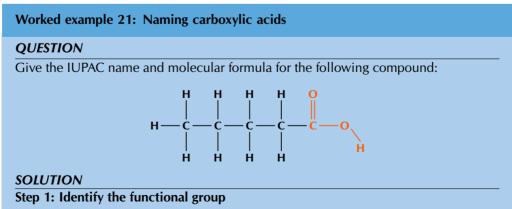
First condense the main chain including the carbonyl group oxygen atom: $\rm CH_3COCHCH_2CH_3$

Then add the side chains on the relevant carbon atoms: CH₃COCH(CH₃)CH₂CH₃



Naming carboxylic acids

Carboxylic acids are characterised by having a carboxyl group, which has the formula –COOH. In a carboxyl group a carbon atom is double-bonded to an oxygen atom (a carbonyl group), and is also bonded to a hydroxyl (alcohol) group. The IUPAC suffix for a carboxylic acid is -oic acid.



The compound has a –COOH group and is therefore a carboxylic acid. The suffix will be -oic acid.

Step 2: Find the longest carbon chain that contains the functional group

There are five carbon atoms in the longest chain that contains the functional group, and only single bonds between carbon atoms. The prefix for this compound is pentan.

Step 3: Number the carbon atoms in the carbon chain

The carbon atoms will be numbered from right to left so that the carboxylic acid functional group has the lowest numbered carbon atom.

Step 4: Look for any branched groups

There are no branched groups in this compound.

Step 5: Combine the elements of the compound's name into a single word in the order of branched groups; prefix, name ending according to the functional group The compound's name is **pentanoic acid**.

Step 6: Reduce the structural representation to the molecular formula

There are 5 carbon atoms, 10 hydrogen atoms and 2 oxygen atoms so the molecular formula is $C_5H_{10}O_2$.

Worked example 22: Naming carboxylic acids

QUESTION

Draw the structural and condensed structural representations for the organic compound **2-ethylhexanoic acid**.

SOLUTION

Step 1: Identify the functional group

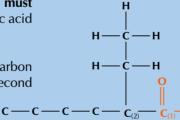
The compound has the suffix -oic acid. It is therefore a carboxylic acid and has a -COOH group. This group can only be on carbon 1 (at the end of the carbon chain).

Step 2: Find the longest carbon chain that contains the functional group

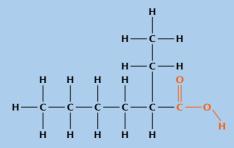
The prefix is hex- therefore there are 6 carbons in the longest chain.

Step 3: Place the functional group as well as any branched groupsRemember that the main carbon chain mustHcontain the functional group. This is hexanoic acidHand not a substituted heptane.H

The –COOH group contains the first carbon atom. The ethyl group is attached to the second carbon atom.



Step 4: Combine this information and add the hydrogen atoms



Step 5: Condense the structural representation

First condense the main chain, including the -COOH functional group: CH₃CH₂CH₂CH₂CH₂CHCOOH Then add the side chains (in brackets) on the relevant carbon atoms: CH₃CH₂CH₂CH₂CH₂CH(CH₂CH₃)COOH

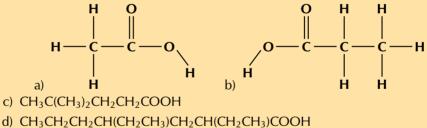
Activity: Building carboxylic acids

Using atomic model kits build the molecules of methanoic acid, ethanoic acid, butanoic acid, pentanoic acid and octanoic acid. If you don't have an atomic model kit remember that you can use jelly tots (or playdough) and toothpicks. Use different colour jelly tots to represent the different atoms and two toothpicks to represent double bonds.

- You should see that all these compounds have a similar formula. Remember, they belong to the carboxylic acid homologous series. What is the general formula for this series?
- Remember that carbon must have four bonds, oxygen must have two bonds and hydrogen can only have one bond. Thinking about this fact, is it possible to have the carboxylic acid (-COOH) group in a position other than the last (or first) carbon atom?

Exercise 4 - 15: Naming carboxylic acids

- 1. Give the structural representation for the following:
 - a) pentanoic acid b) 4-ethyl-7-methyloctanoic acid
 - c) 4,4-diethylheptanoic acid
- 2. Give the IUPAC name for each of the following:



3. More questions. Sign in at Everything Science online and click 'Practise Science'.

Check answers online with the exercise code below or click on 'show me the answer'.

1.27N4 2.27N5

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Naming esters

When an alcohol reacts with a carboxylic acid an *ester* is formed. A new bond is formed between the oxygen atom of the hydroxyl group and the carbonyl carbon atom of the carboxylic acid. The suffix for an ester is -oate.

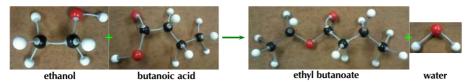


Figure 4.49: The esterification process of ethanol and butanoic acid to ethyl butanoate and water.

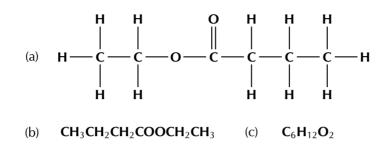
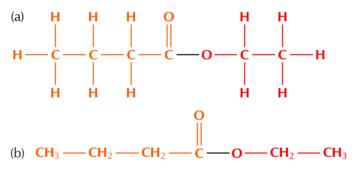




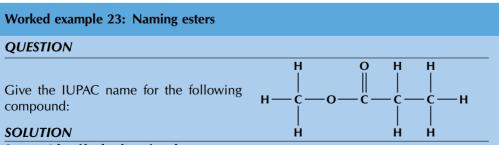
Figure 4.50: The (a) structural, (b) condensed structural and (c) molecular formula representations of ethyl butanoate. (d) An atomic model of ethyl butanoate.

Although the part of the ester from the alcohol (ethyl) is on the right, and the part from the carboxylic acid (butan-) is on the left in Figure 4.51, when naming the structure the part of the name from the alcohol is written first (ethyl butanoate). Don't forget to count the carbon atom in the carbonyl group when determining the number of carbon atoms in the chain.



(c) $CH_3CH_2CH_2COOCH_2CH_3$

Figure 4.51: The (a) structural, (b) semi-structural structural and (c) condensed structural representations of ethyl butanoate.



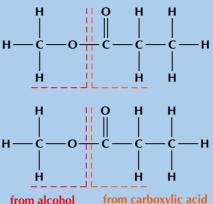
Step 1: Identify the functional group

There is a -C=O (carbonyl) group as well as an oxygen atom bonded to the carbon atom of the carbonyl and another carbon atom. This is therefore an ester and the suffix is -oate.

Step 2: Determine which part is from the alcohol and which is from the carboxylic acid

An ester is a carboxylic acid derivative. Divide the molecule in two with the carbonyl group on one side and the oxygen bonded to two carbon atoms on the other.

The part containing the oxygen atom bonded to two different carbon atoms was formed from the alcohol and is on the left here. The part containing the carbonyl group was formed from the carboxylic acid and is on the right here.



Step 3: Number the carbon atoms on the carbon chains

There is only one carbon atom in the left-hand chain (from the alcohol). Therefore this will be methyl. There are three carbon atoms in the right-hand chain (from the carboxylic acid) therefore the prefix will be propan-.

Step 4: Combine the elements of the compound's name into a single word in the order of chain from the alcohol; prefix (from chain containing carbonyl functional group), name ending according to functional group

The compound's name is methyl propanoate.

Worked example 24: Naming esters

QUESTION

Draw the structural and condensed structural representations for the organic compound **ethyl hexanoate**.

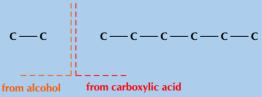
SOLUTION

Step 1: Identify the functional group

The compound has the suffix -oate. It is therefore an ester and has a -C=O (carbonyl) group as well as an oxygen atom bonded to the carbon atom of the carbonyl and another carbon atom.

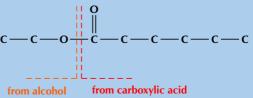
Step 2: Determine which part is from the alcohol and which is from the carboxylic acid

The ethyl tells us that there are two carbon atoms in the part of the chain from the alcohol. The prefix hex- tells us that there are six carbon atoms from the part of the chain from the carboxylic acid.

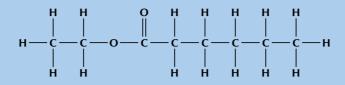


Step 3: Place the functional group as well as any branched groups

The oxygen atom bonded to two different carbon atoms is located between the two sections. The -C=O (carbonyl) group is located at the first carbon atom of the carboxylic acid chain.



Step 4: Combine this information and add the hydrogen atoms



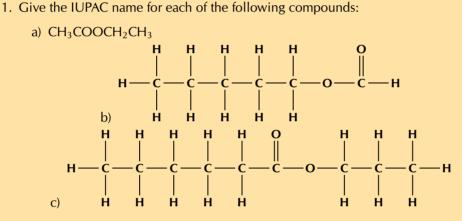
Step 5: Condense the structural representation

Condense the part of the compound that came from the carboxylic acid first, so start from the right here: $CH_3CH_2CH_2CH_2CH_2COO$

The first O is for the -C=O, the second is from the -O-. Now condense the part that came from the alcohol, starting from the -O-:

CH₃CH₂CH₂CH₂CH₂COOCH₂CH₃

Exercise 4 – 16: Naming esters



- 2. Give the structural representations for the following esters:a) heptyl propanoate b) methyl octanoate c) hexyl pentanoate
- 3. More questions. Sign in at Everything Science online and click 'Practise Science'.

Check answers online with the exercise code below or click on 'show me the answer'. 1. 27N6 2. 27N7

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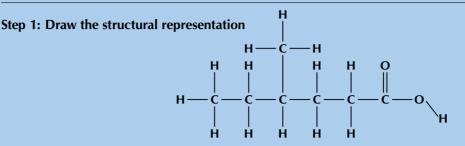
Worked example 25: Naming carbonyl compounds

QUESTION

Give the IUPAC name for the following compound: CH₃CH₂CH(CH₃)CH₂CH₂COOH

(Remember that the side groups are shown in brackets after the carbon atom to which they are attached)

SOLUTION



Step 2: Identify the functional group

The compound has a -COOH functional group. It is therefore a carboxylic acid and the suffix is -oic acid.

Step 3: Find the longest carbon chain containing the functional group

There are six carbon atoms in the longest chain containing the functional group. The prefix for this compound is hexan-.

Step 4: Number the carbon atoms in the carbon chain

The carbon atoms should be numbered from right to left so that the carboxylic acid functional group has the lowest numbered carbon atom.

Step 5: Look for any branched groups, name them and give their position on the carbon chain

There is a branched group attached to the fourth carbon atom. This group has only one carbon atom and is therefore a methyl group (4-methyl).

Step 6: Combine the elements of the compound's name into a single word in the order of branched groups; prefix; name ending according to the functional group The compound's name is **4-methylhexanoic acid**.

Worked example 26: Naming carbonyl compounds

QUESTION

Give the IUPAC name for the following compound: CH₃COOCH₂CH₂CH₂CH₂CH₃

SOLUTION

Step 1: Identify the functional group

The compound has a -COO functional group. It is therefore an ester and the suffix will be -oate. This can also be shown as:

$CH_3\ddot{C}-O-CH_2CH_2CH_2CH_3$

Step 2: Determine which part is from the alcohol and which is from the carboxylic acid

The left half of the compound contains the carbonyl group and is therefore from the carboxylic acid. The right half of the compound must be from the alcohol.

CH₃C-O-CH₂CH₂CH₂CH₂CH₃

Step 3: Determine the number of carbon atoms in each chain

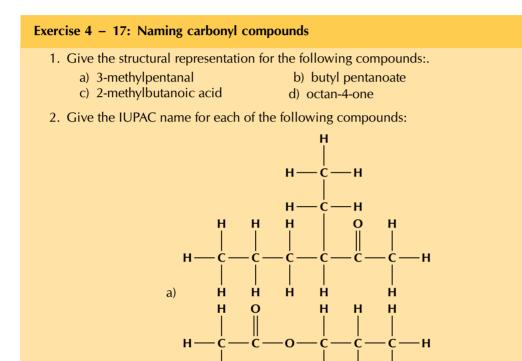
There are 2 carbon atoms in the part that contains the C = O group (from the carboyxlic acid), therefore the prefix is ethan-. There are 4 carbon atoms in part of the chain without the carbonyl group (from the alcohol), which is therefore butyl.

Step 4: Look for any branched groups, name them and give their position on the carbon chain

There are no branched groups.

Step 5: Combine the elements of the compound's name into a single word in the order of name of chain from the alcohol; prefix (from chain containing carbonyl functional group); suffix

The compound's name is **butyl ethanoate**.



н c) CH₃CH₂CH₂CHO d) HCOOH

3. More questions. Sign in at Everything Science online and click 'Practise Science'. Check answers online with the exercise code below or click on 'show me the answer'. 1.27N8 2.27N9

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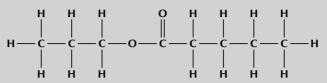
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Activity: Building molecules

Using atomic model kits build molecules of butane, but-1-ene, but-1-yne, butan-1-ol, butanoic acid, butyl butanoate, butan-2-one, butanal. If you don't have an atomic model kit remember that you can use jelly tots (or playdough) and toothpicks. Use different colour jelly tots to represent the different atoms and extra toothpicks to represent double and triple bonds.

• Identify the functional group in each of these molecules. Move the functional group around the molecule. You should find that you can do so with but-1-ene, but-1-yne and butan-1-ol. It will not be possible with butanoic acid and there is no functional group to move in butane.

- Can you see that if you move the carbonyl group in butan-2-one you will either still get butan-2-one or you will get butanal? Similarly, when moving the carbonyl group in butanal you can only get butanal or butan-2-one.
- Build a model of the molecule below:



Compare this to butyl butanoate. What differences are there between these two molecules? What similarities are there? What is the name of the new molecule?

• Continue by building different compounds for your friends. Make them identify the functional group, the number of carbon atoms and therefore the name of the compound.

Exercise 4 – 18: IUPAC naming

1. Study the table below and answer the questions that follow:

	A	В	С
	Compound	Functional group	Number of carbon atoms
1	e.g. methane	e.g. alkane	e.g 1
2	propanoic acid	alkyne	8
3	2-chloroethane	ketone	4
4	1-octanal	carboxylic acid	6
5	3-heptyne	aldehyde	2
6	butanone	ester	6
7	3-hexene	haloalkane	1 and 5
8	1-hexanol	alkene	3
9	methyl pentanoate	alcohol	7

a) Match the compounds in column A with the correct functional group in column B. For example methane is an alkane: **A1**, **B1**.

- b) Match the compounds in column A with the correct number of carbon atoms in column C. For example methane has one carbon atom in its longest chain: A1, C1.
- 2. Match the structural representation in column A with the condensed structural representation (column B) and IUPAC name (column C).

	Α	В	С
	Structure	Condensed	IUPAC name
1	H H H H—C—C—C—H H H H	CH ₃ CH(I)CH ₃	ethyl methanoate
	нпп		euryr meuranoate
	н—с—с≡с—н		
2	H	$CH_3CH_2CH_3$	propanone
	н о н н—с—с—с—н		
3		CH ₃ COCH ₃	propane

	A	В	С
	Structure	Condensed	IUPAC name
	Н Н О H—с—с—с—он		
4	H H	HCOOCH ₂ CH ₃	propyne
	H I H H—C—C—C—H		
5		CH ₃ CCH	propanal
6		CH_3CHCH_2	2-iodopropane
7	н н	CH ₃ CH ₂ CHO	propanoic acid
	H H O HCCH		
8	НН	CH ₃ CH ₂ COOH	propene

3. Fill in the gaps in the table below:

IUPAC name	Functional	Condensed	Structural
Папе	group		ннно
		CH ₃ CH ₂ CH ₂ CHO	н—с—с—с—с—п н н н
			Н О—Н H—С—С—Н
ethanol			H H
	carboxylic acid	CH ₃ CH ₂ CH(CH ₃)CH ₂ COOH	
2-methyl pent-2-ene		CH ₃ C(CH ₃)CHCH ₂ CH ₃	
	alkane		H H-C-H H H H-C-C-C-H H H H H
	ester	CH ₃ COOCH ₂ CH ₂ CH ₃	
butanone	ketone		ннн
1-pentyne			H H H H H—c≡c—c—c—c—H H H H H
	alkyl halide	CH ₂ (Cl)CH ₂ CH ₃	