# *Higher Chemistry*

*Topic 5*:

*Organic 1*

# Study Guide 2

# Structures & Naming

# NAMING MOLECULES 5.2

## ⊙ *Introduction*

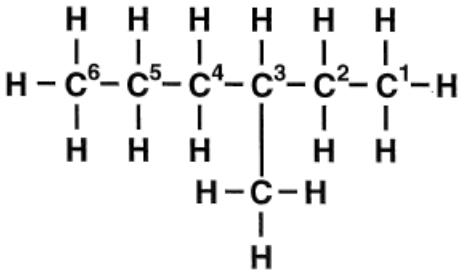
As you will know from previous work, alkanes and alkenes mainly have chain-like molecules with names based on the number of carbon atoms in the chain as well as the size and position of branches. Alcohols were also used to show how the presence of a functional group can influence the numbering system.

*This lesson largely revises the principles behind naming and how they can be applied in more complex molecules*

## ① *Naming and Drawing Alkanes*

*This activity deals with how to name branched alkanes using systematic names, i.e. names that follow a very definite system which is based on the structure of the molecule.*

Consider this molecule



Remember that the naming system begins with the ***back*** of the name.

**1.** Main Chain: ⟶ ***hexane***

**2.** Side Group: ⟶ ***methyl***

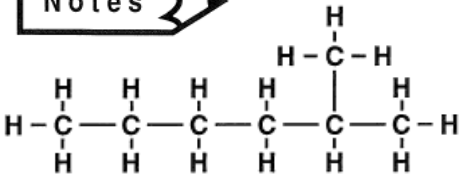
**3.** Position: ⟶ ***3***

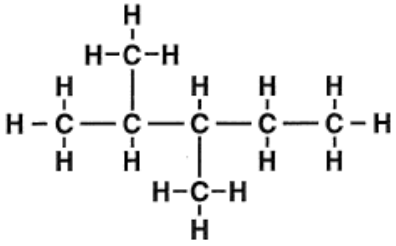
So the complete name is ***3-methylhexane***. Notice that there are ***no spaces in the name*** and there is a ***hyphen between number and letters***.

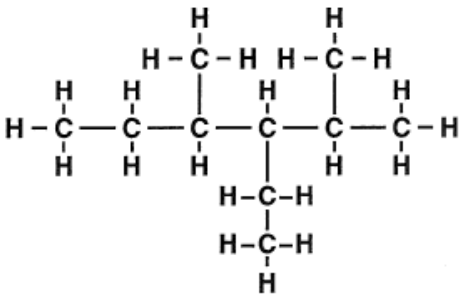
What to do

Notes

**1.** Work out the systematic name for each of these molecules.







**2.** Work out the full structural formula for each of the following.
(***Hint:*** start at the ***back*** and draw the main chain first.)

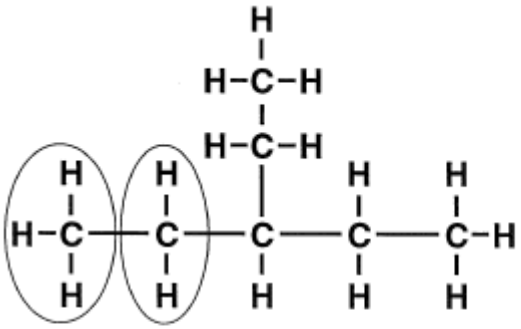
***a)*** 3-methylpentane ***b)*** 4,4-dimethyloctane ***c)*** 5-ethyl-2-methylheptane

Full structural formulae, especially for large molecules, occupy a lot of space and can be time-consuming to draw. Quite often a shorter version of the structure will do just as well.

*This activity is about writing and using shortened structural formulae for alkanes.*

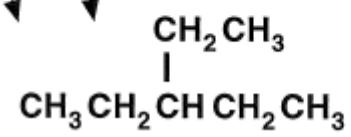
Full structural formulae, especially for large molecules, occupy a lot of space and can be time-consuming to draw. Quite often a shorter version of the structure will do just as well.

The upper diagram shows the full structural formula for 3-ethylpentane.



full structural formula

The lower diagram shows a shortened structural formula.



shortened structural formula

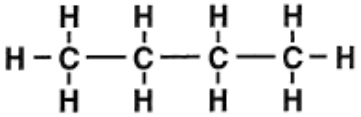
Notice that no bonds are shown in the main chain. Only the bond to the branch is needed.

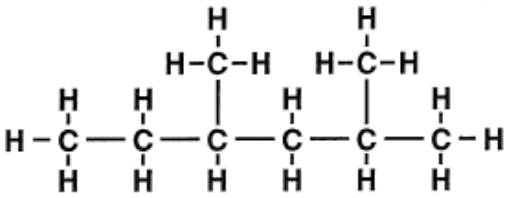
Each carbon in the chain is still shown separately along with any other atoms attached. Thus the end group becomes $CH_3$ , while the next group in the chain is $CH_2$ , and so on.

What to do

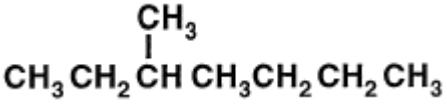
Notes

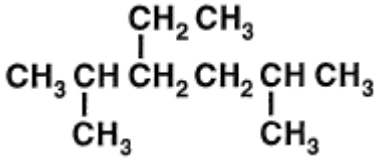
**1.** Work out the shortened structural formula for each of these molecules.





**2.** Work out the systematic name from the shortened structural formula for each of these molecules.





**3.** Work out the shortened structural formula for each of the following. (***Hint:*** start at the ***back*** and draw the main chain first.)

***a)*** 3-methylpentane ***b)*** 2,4-dimethylhexane

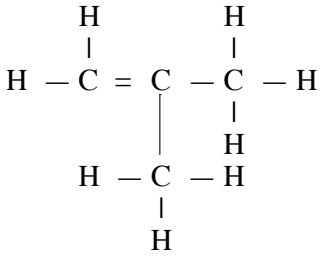
## ② *Naming and Drawing Alkenes*

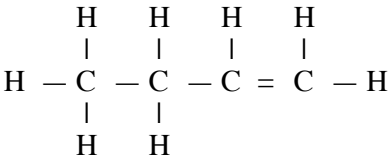
Alkene structures can differ in two ways, branching and the position of the double bond. Both of these possibilities have to be taken into account in the naming system.

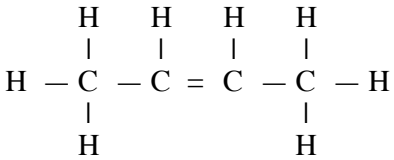
*This activity considers how to use systematic names to indicate both the positions of side branches and the position of the double bond in an alkene structure.*

The following structural formulae all represent alkenes with the molecular formula $C_4H_8$ but they are clearly not the same. Such molecules are examples of ***isomers***.

***Isomers*** are compounds which have the ***same*** *molecular formula* but ***different*** *structural formulae.*







Think

Think about how you would name the isomers above.

- From which end of the chain should an alkene structure be numbered?
- Which carbon atom decides the number for the double bond position?
- Where does the position number for the double bond come in the name?
- How is the number separated from the letters in the name?
- How would you name the three alkene isomers shown above?
- Why would but-3-ene ***not*** be yet another straight-chain isomer?
- Why would a methyl branch at carbon 1 in propene not give yet another branched-chain isomer?

Notes

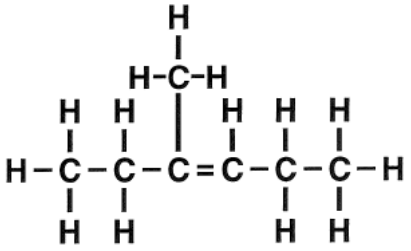
What to do

**1.** Draw the full and shortened structural formulae for

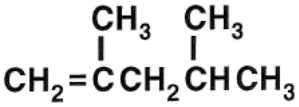
***5-methyloct-2-ene***

Notes

**2.** Work out the systematic name and draw the shortened structural formula for the following molecule

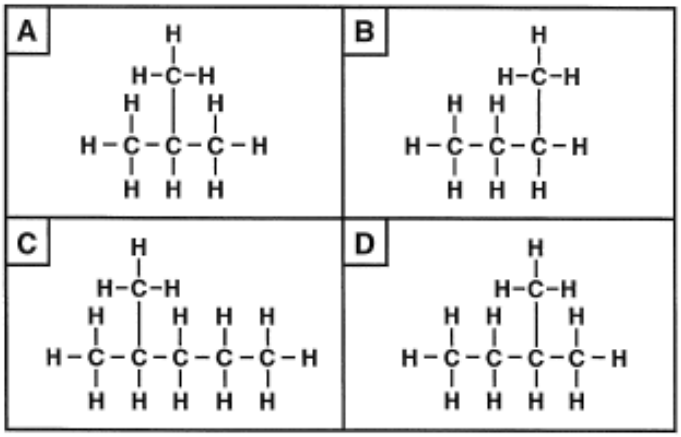


**3.** Work out the systematic name and draw the full structural formula for the following molecule



# CHECK TEST 5.2A

***Questions 1 and 2 refer to the following structural formulae.***




***Q1.*** Which structural formula represents a straight-chain hydrocarbon?

***Q2.*** Which is the structural formula for 2-methylpentane?

***Q3.*** What is the shortened structural formula for 4-ethyl-3-methyloctane?

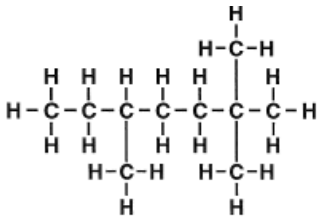
**A** $CH_3CH_2CH_2CH_2CH(CH_2CH_3)CH(CH_3)CH_2CH_3$

**B** $CH_3CH_2CH_2CH(CH_3)CH_2CH(CH_2CH_3)CH_2CH_3$

**C** $CH_3CH_2CH(CH_2CH_3)CH_2CH_2CH(CH_3)CH_2CH_3$

**D** $CH_3CH_2CH(CH_3)CH(CH_2CH_3)CH_2CH_2CH_2CH_3$

***Q4.*** The systematic name for this hydrocarbon is



**A** 3-methyl-2,2-dimethylheptane

**B** 2,2,3-trimethylheptane

**C** 2-ethyl-5-methylheptane

**D** 2,2,5-trimethylheptane

***Q5.*** What is the shortened structural formula for hept-2-ene?

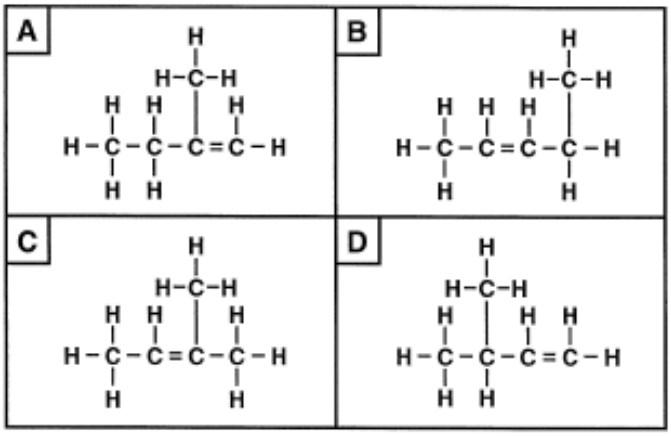
**A** $CH_3CH_2CH{=}CH\,CH_2CH_2CH_3$

**B** $CH_3CH_2CH_2CH{=}CH\,CH_2CH_3$

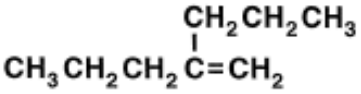
**C** $CH_3CH_2CH_2CH_2CH{=}CH\,CH_3$

**D** $CH_3CH_2CH_2\,CH_2CH_2CH{=}CH_2$

***Q6.*** What is the full structural formula for 3-methylbut-1-ene?




***Q7.*** The systematic name for this hydrocarbon is



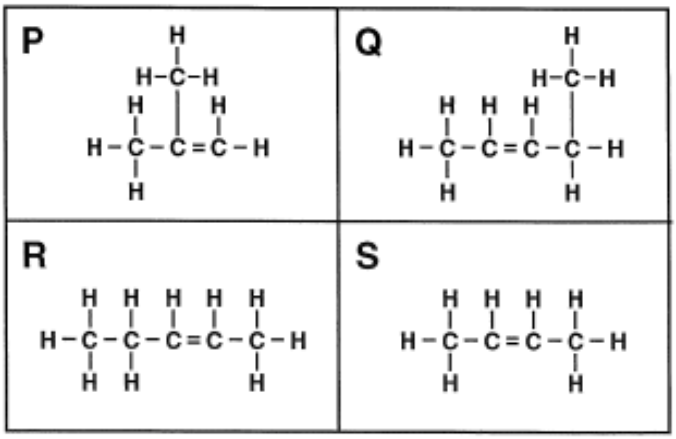
**A** 4-methylhept-4-ene

**B** 2-propylpent-1-ene

**C** 1, 1-dipropylethene

**D** 2-propyloct-4-ene

***Q8.*** Which of the following are isomers?



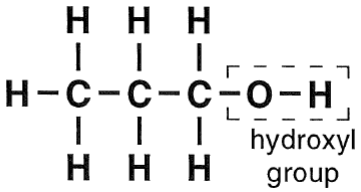
# ③ *Naming and Drawing Alkanols*

Any molecule containing a hydroxyl group —OH can be considered an alcohol. The acohols based on saturated chains, based on alkane molecules, are called alkanols.

*This activity revises the names and structures of simple straight-chain alkanols.*

There are several ways to represent the formula of an alkanol. In each case it is useful to show the hydroxyl group separately because it is this group which gives alcohols their characteristic chemical reactions. Without the hydroxyl group such molecules would not function as alcohols.

full structural formula




shortened structural formula

$CH_3CH_2CH_2OH$

functional molecular formula

$C_3H_7OH$

Think

Think about the three formulae shown above.

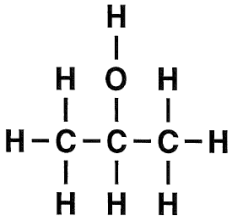
- Which alkanol do all three of these formulae represent?
- Why is the hydroxyl group shown separately in each one?
- Which type of formula gives the most detail?

The molecular formula for this molecule is $C_3H_8O$

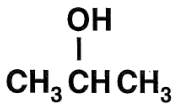
- Draw the structure for another molecule that has the same molecular formula but does not contain a hydroxyl group.
- Is this molecule an isomer of the alkanol above?
- Why would an ordinary molecular formula not be very helpful?

Propanol is the smallest alkanol molecule which can have isomers. The isomerism arises from the possibility of putting the hydroxyl group in different positions.

Instead of having the hydroxyl on the end carbon, the isomer of propanol in the diagram has the hydroxyl group attached to the second carbon. This is shown in the name by inserting the number 2 (with hyphens on each side) just before the 'ol' ending. The name propan-2-ol is read as 'propan-two-ol'.



OR



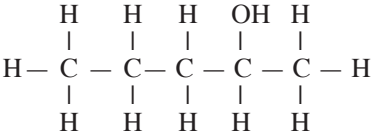
propan-2-ol

What to do

Notes

**1.** Draw the full and shortened structural formulae for ***heptan-4-ol***

**2.** Work out the systematic name and draw the shortened structural formula for this molecule



**3.** Work out the systematic name and draw the full structural formula for the following molecule

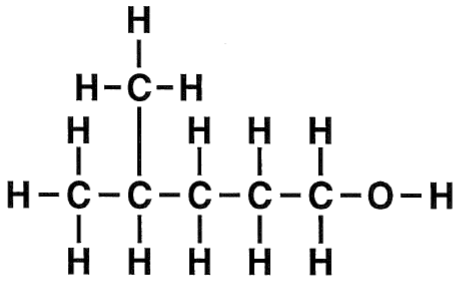
**$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2OH$**

Just as an alkane can have a branched structure, so also the hydrocarbon chain in an alkanol molecule can be branched. The systematic name for a branched alkanol must therefore include the position number for both the hydroxyl group and the branch.

*This activity considers how to use systematic names to indicate both the position of the functional group and the position of a branch in branched-chain alkanol.*

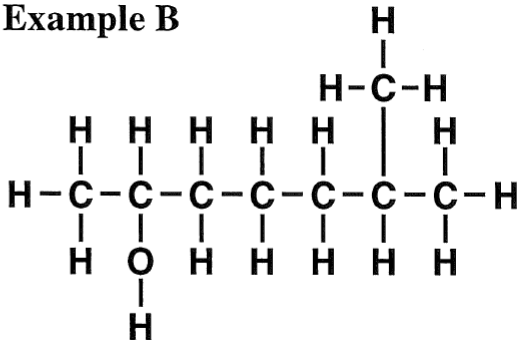
The main chain in a branched alkanol is determined by the longest chain which includes the hydroxyl functional group. The carbon atoms are then numbered from the end which is nearer the hydroxyl group. You can see this in example A, an isomer of $C_6H_{13}OH$.

**Example A**



4-methylpentan-1-ol

**Example B**



Think

Think first about the molecule in example A.

- Why is the name based on pentanol despite there being 6 carbon atoms in the molecule? (Clue: How many C atoms are in the longest chain?)
- Why is the main chain numbered from the right and not from the left?
- Why are there **two** numbers in the name?

Now think first about the molecule in example B.

- How many C atoms are in the longest chain that includes the OH group?
- What alkanol, therefore, must the name be based upon?
- Which end of the main chain is nearer the hydroxyl? What number position does this give the hydroxyl group?
- What position number does this give the methyl group?

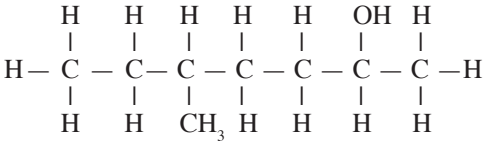
Notes

What to do

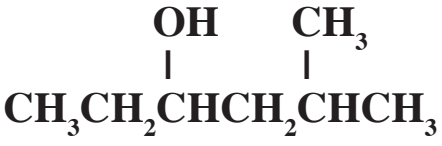
**1.** Draw the full and shortened structural formulae for ***2-methylpentan-1-ol***

Notes

**2.** Work out the systematic name and draw the shortened structural formula for this molecule



**3.** Work out the systematic name and draw the full structural formula for the following molecule



# CHECK TEST 5.2B

***Q1.*** What is the general formula for the alkanol series?

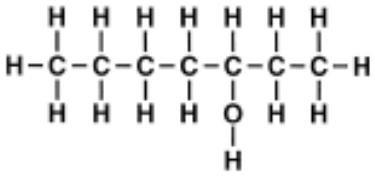
**A** $C_nH_{2n+2}OH$

**B** $C_nH_{2n-2}OH$

**C** $C_nH_{2n-1}OH$

**D** $C_nH_{2n+1}OH$

***Q2.*** The systematic name for this molecule is



**A** octan-3-ol

**B** heptan-5-ol

**C** octan-5-ol

**D** heptan-3-ol

***Q3.*** Which of the following is ***not*** a possible name of $C_6H_{13}OH$

**A** hexan-4-ol

**B** hexan-3-ol

**C** hexan-2-ol

**D** hexan-1-ol

***Q4.*** The systematic name for this molecule is

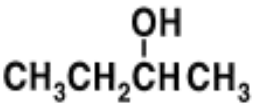
**A** propan-1-ol

**B** propan-4-ol

**C** butan-1-ol

**D** butan-4-ol

***Q5.*** Which of the following is an isomer of this molecule?



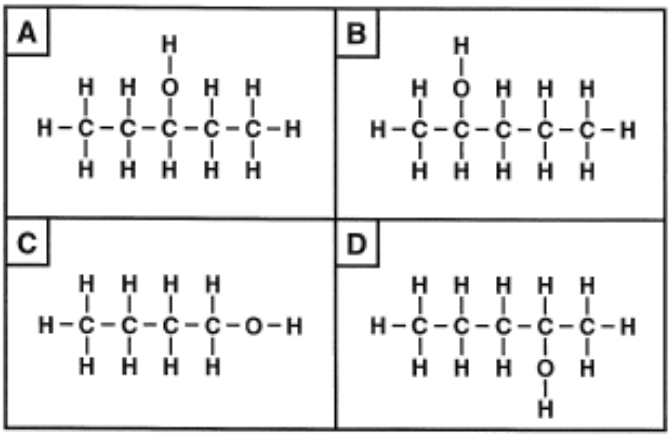
**A** propan-1-ol

**B** butan-1-ol

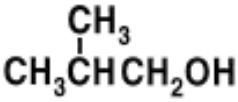
**C** propan-2-ol

**D** butan-2-ol

***Q6.*** Which of the following is an isomer of pentan-2-ol?




***Q7.*** The systematic name for this molecule is



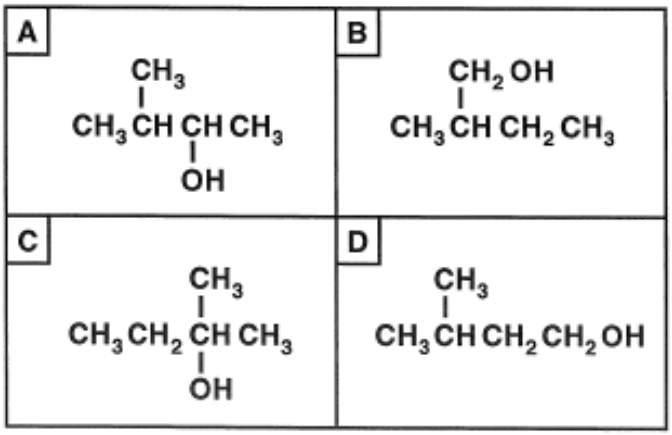
**A** 2-methylbutan-1-ol

**B** 3-methylbutan-1-ol

**C** 2-methylpropan-3-ol

**D** 2-methylpropan-1-ol

***Q8.*** Which structure is 2-methylbutan-2-ol?



## ③ *Other Alcohol Structures*

Although all alcohols have similar chemical reactions, there are also differences depending on the detailed structure of the molecule, especially the part around the hydroxyl group. In addition to straight-chain and branched structures it is also possible to have rings structures and alcohols with more than one hydroxyl group.

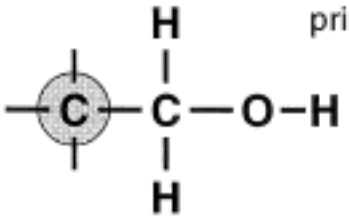
*This lesson topic looks in more detail at a variety of alcohol structures.*

Alcohols can be classified into three types depending on the ***number of carbon atoms joined to the carbon which has the hydroxyl group***.

In a ***primary alcohol*** no more than ***one*** carbon atom is joined directly to the carbon bonded to the hydroxyl group.

***'hydroxyl group at end of chain'*** **eg** *propan-1-ol*

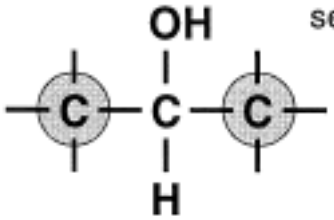
***mild oxidation:*** ⟶ *aldehyde* ⟶ *carboxylic acid*




In a ***secondary alcohol*** there are ***two*** carbons attached to the carbon bonded to the hydroxyl group.

***'hydroxyl group in middle of chain'*** **eg** *propan-2-ol*

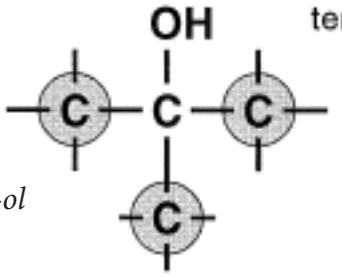
***mild oxidation:*** ⟶ *ketone*




In a ***tertiary alcohol*** there are ***three*** carbons attached to the carbon bonded to the hydroxyl group.

***'hydroxyl group in middle of chain at branch site'*** **eg** *2-methylpropan-2-ol*

***mild oxidation:*** *no product*




What to do

Notes

**1.** Draw the structural formulae for an alcohol isomer of $C_5H_{11}OH$ which is:

***a)*** primary ***b)*** secondary ***c)*** tertiary

**2.** Work out the systematic name of each structure you have drawn.

Think

Consider the three pentanol structures you have drawn to help you think about the following questions.

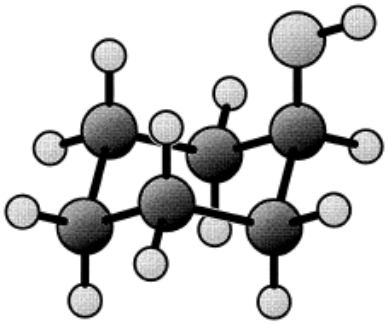
- Which type of alcohol (primary, secondary or tertiary) always has the hydroxyl group at the ***end of a chain***?
- Which type of alcohol (primary, secondary or tertiary) always has the hydroxyl group at a non-branching position ***along a chain***?
- Which type of alcohol (primary, secondary or tertiary) always has the hydroxyl group at a ***branching position*** in a chain?

Notes

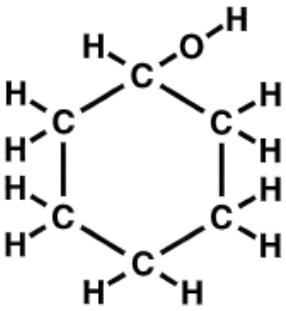
A cycloalkanol is essentially a cycloalkane in which a hydrogen atom in the molecule has been replaced by a hydroxyl group.

A typical example is ***cyclohexanol*** and this is illustrated in the diagram.

The name is simply taken from the corresponding alkanol with the prefix 'cyclo' written in front. Just where you show the hydroxyl group in the structural formula is a matter of choice.



*molecular model*



*structural formula*

**Think**

Think about the name of ***cyclohexanol*** in relation to its structure.

- Which part of the name indicates that the ***hydroxyl*** group is present?
- Which part of the name indicates that it has a ***ring*** structure?
- Which part of the name tells you that all of the bonds between the carbon atoms in the ring are ***single bonds***, that it is ***saturated***?
- Which part of the name means that the ring has ***six*** carbon atoms?

Now think about the structure and formula of the molecule.

- Why can cyclohexanol be considered a ***secondary*** alcohol?
- Is it possible for a cycloalkanol to be a ***primary*** alcohol? a ***tertiary*** alcohol? (If yes, draw an example of each).
- What is the functional molecular formula for cyclohexanol?
- Why is cyclohexanol ***not*** an isomer of hexanol?

**Notes**

**What to do**

**1.** Draw the full structural formulae for as many cycloalkanol isomers as possible for each of the following:

***a)*** $C_4H_7OH$ ***b)*** $C_5H_9OH$

**Notes**

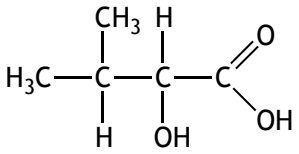
**2.** For each isomer drawn, try to work out the systematic name and state whether it is a *primary*, *secondary* or *tertiary* alcohol.

**Think**

Consider the various isomers you have drawn and named.

- Is it possible to have an alcohol isomer that is a ***primary*** alcohol. Is it a cycloalkanol? Can it be easily named?
- Is it possible to have an alcohol isomer that is a ***secondary*** alcohol. Is it a cycloalkanol? Can it be easily named?
- Is it possible to have an alcohol isomer that is a ***tertiary*** alcohol. Is it a cycloalkanol? Can it be easily named?

The previous examples will have introduced the need to sometimes consider part of a molecule as being a substituent 'group' rather than the main part of the molecule. With alcohols, you will also see '***hydroxy***' used rather than the expected '-***ol***' ending.

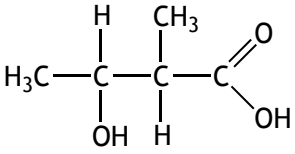


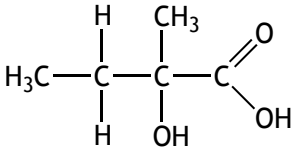
You will often be expected to use an example of a named molecule and use that to work out the name of a similar molecule. For example, the molecule opposite is named as

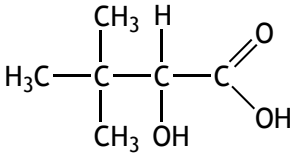
***2-hydroxy-3-methylbutanoic acid***

**What to do**

By examining the example above, work out the systematic names of the following 3 molecules







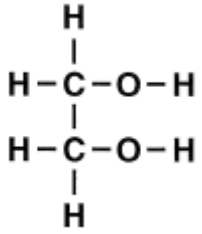
There are some alcohols that have more than one hydroxyl group in the molecule. For example, ***glycol***, which is used as the antifreeze in car radiators, and ***glycerol***, which is found in a variety of foods, such as soft ice-cream.

The alcohol used in ordinary car antifreeze has ***two*** *hydroxyl* groups and for this reason is known as a ***dihydric*** alcohol or ***diol***. Its common name is *glycol*, but this says little about its structure.

The systematic name is ***ethane-1,2-diol***.

Two numbers are needed in the name to describe the positions of the ***two*** hydroxyl groups. Notice that 'di' now appears in front of 'ol' ('di' = 2, 'ol' = *hydroxyl* group).

With two carbon atoms in the molecule, the systematic name is based on ***ethane***. In this case the final 'e' of ethane is ***not*** dropped in the systematic name because it is not followed by a vowel.



*ethane-1,2-diol*

The alcohol commonly known as ***glycerol*** (sometimes called ***glycerine***) is not only widely used in the production of foodstuffs, it is also used by plants and animals to produce ***fats & oils*** as long term ***energy storage*** molecules. It has the systematic name ***propane-1, 2, 3-triol***.

**What to do**

Collect a box of model atoms and construct a model of ***propane-1, 2, 3-triol*** to see what the real shape of this molecule is like.

**Think**

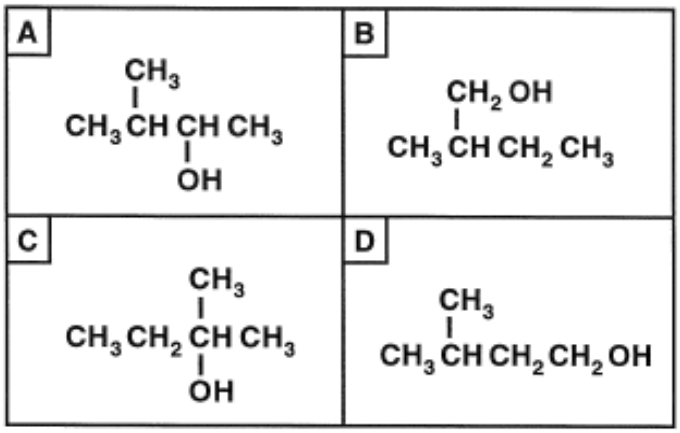
Think about the structure and name of ***propane-1, 2, 3-triol*** (*glycerol*)

- Why can this alcohol be described as ***trihydric***?
- Why is the 'e' retained in the systematic name for *glycerol*?
- Why is it important to have three numbers in this name?
- What is the difference in use of hyphens and commas in this name?

**Notes**

# CHECK TEST 5.2c

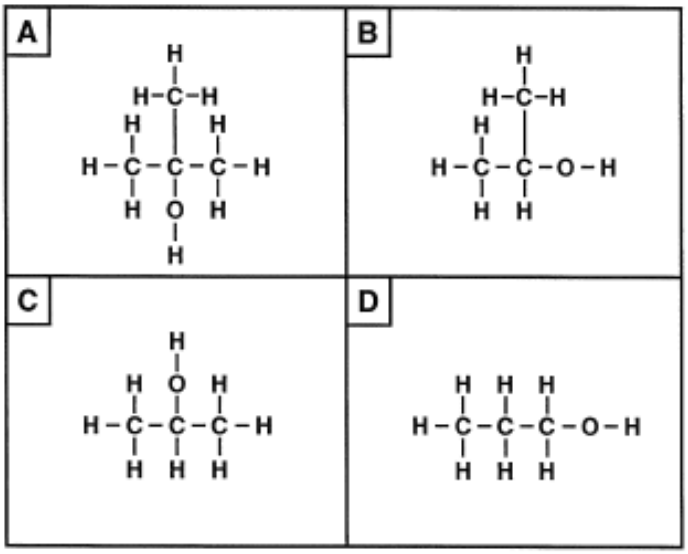
***Questions 1 and 2 refer to the following structural formulae.***



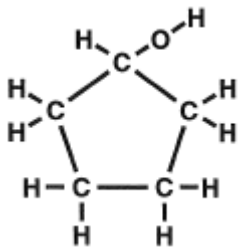

***Q1.*** Which is a secondary alcohol?

***Q2.*** Which is a tertiary alcohol?

***Q3.*** Which of the following structures is a primary alcohol?




***Q4.*** The systematic name for this molecule is



**A** butanol

**B** cyclobutanol

**C** pentanol

**D** cyclopentanol

***Q5.*** The structural formula of a trihydric alcohol has three

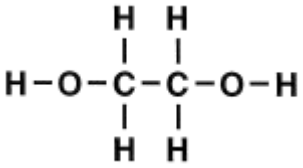
**A** carbon atoms

**B** hydrogen atoms

**C** hydroxyl groups

**D** methyl groups

***Questions 6 and 7 refer to the following structural formulae.***



***Q6.*** This molecule is an example of a

**A** diol

**B** secondary alcohol

**C** diatomic compound

**D** branched alcohol

***Q7.*** The correct systematic name for the molecule is

**A** ethane-1, 1-diol

**B** ethane-1, 2-diol

**C** ethan-1, 1-diol

**D** ethan-1, 2-diol

***Q8.*** Which of the following is an example of a secondary alcohol?

**A** ethanol

**B** cyclobutanol

**C** methanol

**D** butan-1-ol

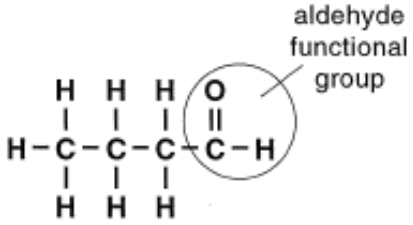
# ④ *Aldehydes & Ketones*

***Oxidation*** of ***primary*** and ***secondary*** alcohols produces ***aldehydes*** and ***ketones*** respectively. Both aldehydes and ketones are examples of ***carbonyl*** compounds, both of them containing the ***carbonyl group***, C=O.

*This activity considers the structures and systematic names of the alkanal series of aldehydes and the alkanone series of ketones.*

An ***alkanal*** is a compound which contains the ***carbonyl*** group at the ***end position*** of a hydrocarbon chain in which all the carbon atoms are linked by ***single bonds***.

The most useful formulae for alkanals are full structural formulae and shortened structural formulae.




Notice how ***the aldehyde functional group includes the end hydrogen*** as well as the entire ***carbonyl*** group. In this example, the main chain contains 4 carbon atoms.

In the shortened structural formula, the aldehyde functional group is written as ***CHO***. (To have written COH would have led to confusion with the hydroxyl group in alcohols.)

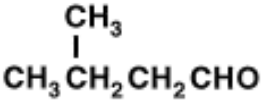
$CH_3CH_2CH_2CHO$

The systematic name is based on the corresponding alkane with the ending changed to '***al***'. (This has to be written clearly to avoid being confused with the 'ol' ending of an alcohol name.)

***butanal***

The main chain in an alkanal molecule is always the longest carbon chain which includes the functional group. Because the functional group, ***CHO***, ***can only occur at the end of a chain*** there is no need for a number in front of the '***al***' in the systematic name.

The carbon atom in the functional group is always number one in the main chain, but its number does ***not*** appear in the name. Numbers are only required for branch positions.

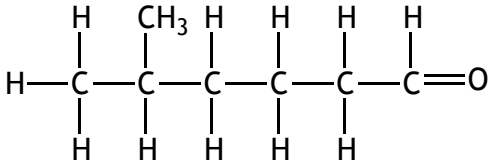


***3-methylbutanal***

**What to do**

**1.** Draw the full and shortened structural formulae for ***2-methylpropanal***

**2.** Work out the systematic name and draw the shortened structural formula for this molecule



**3.** Work out the systematic name and draw the full structural formula for the following molecule

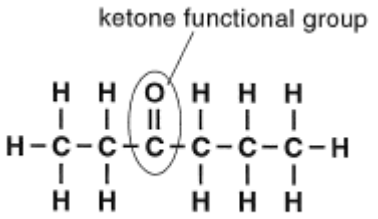
$$CH_3CH_2CHCH_2CH_2CH_2CH_2CHO$$

**Notes**

*This activity considers how to apply systematic names to the alkanone family of ketones.*

An ***alkanone*** is a compound which contains the carbonyl group at a position within a hydrocarbon chain where all the carbon atoms are linked by ***single*** bonds.

The ketone functional group is simply the carbonyl group by itself. The ***carbonyl carbon counts*** as one of the carbon atoms in the main chain. In this example, the main chain contains 6 carbon atoms.




In the shortened structural formula, the ketone functional group is written as CO. It is assumed that you understand that there is a ***double bond*** between the carbon atom and the oxygen atom, although it is ***not shown***.

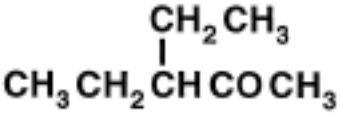
$CH_3CH_2COCH_2CH_2CH_3$

The systematic name is based on the corresponding alkane with the ending changed to '***one***'. For propanone and butanone, no number is needed in the name. From pentanone onwards, alternative positions are possible for the carbonyl group and the position number is inserted in the name just before the '***one***' ending.

***hexan-3-one***

The main chain in an alkanone molecule is always the ***longest carbon chain which includes the functional group***. The main chain is then numbered from the end ***nearest*** to the carbonyl group.

When branching occurs in the molecule, then the systematic name may require two numbers, one for the branch and the other for the carbonyl group if there are five or more carbon atoms in the main chain.



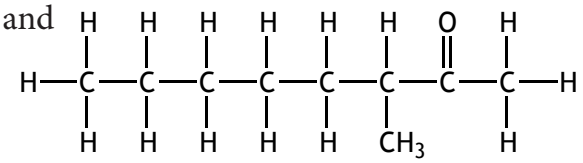
***3-ethylpentan-2-one***

What to do

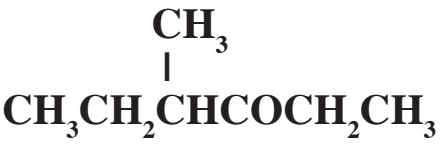
**1.** Draw the full and shortened structural formulae for

***2-methylhexan-2-one***

**2.** Work out the systematic name and draw the shortened structural formula for this molecule



**3.** Work out the systematic name and draw the full structural formula for the following molecule



Think

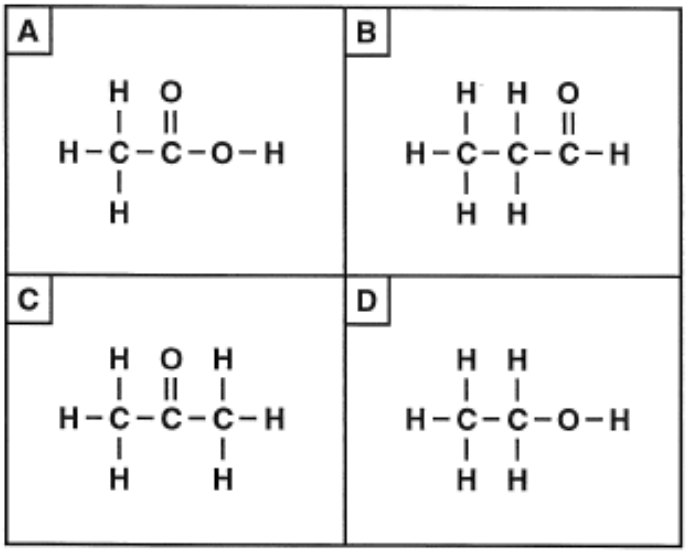
Think about ketone structures.

- Why is propanone the smallest possible ketone structure?
- What aldehyde is an isomer of propanone?
- Why do neither of these compounds require a number in their names?
- What structurally distinguishes a ketone from an aldehyde?

Notes

# CHECK TEST 5.2D

***Questions 1 to 4 refer to the following structural formulae.***



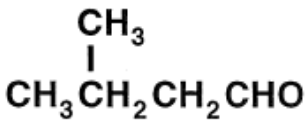

***Q1.*** Which molecule is an alkanol?

***Q2.*** Which molecule is an alkanal?

***Q3.*** Which molecule is an alkanone?

***Q4.*** Which molecule is an alkanoic acid?

***Q5.*** The systematic name for this molecule is



**A** 2-methylbutanal

**B** 2-methylbutanone

**C** 3-methylbutanal

**D** 3-methylbutanone

***Q6.*** The systematic name for this molecule is

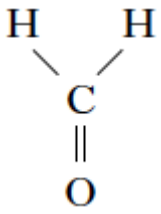
**A** pentan-2-al

**B** pentan-2-one

**C** pentan-4-al

**D** pentan-4-one

***Q7.*** The systematic name for this molecule is



**A** methanol

**B** methanal

**C** methanone

**D** methanoic acid

***Q8.*** Which of the following compounds is an alkanone?

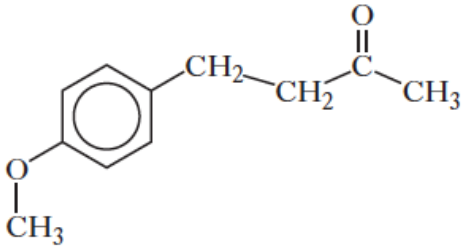
**A** $CH_3CH_2CHO$

**B** $CH_3COOCH_3$

**C** $CH_3COCH_3$

**D** $CH_3COOH$

***Q9.*** A compound with the following structure is used in perfumes to help provide a sweet, fruity fragrance.



This compound can be classified as

**A** an aldehyde

**B** a ketone

**C** a carboxylic acid

**D** an ester

***Q10.*** Which of the following organic compounds is an isomer of hexanal?

**A** 2-methylbutanal

**B** 3-methylpentan-2-one

**C** 2,2-dimethylbutan-1-ol

**D** 3-ethylpentanal

## ④ *Acids & Esters*

As with alkanes, alkanols, and other homologous series, it is possible to have straight chain structures and branching structures in the carbon chain part of the molecule.

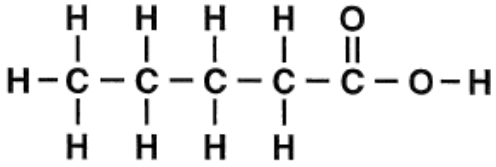
*This activity considers the structures, formulae and systematic names of some of the members of the alkanoic acid family.*

The ***alkanoic acids*** are compounds which contains the ***carboxyl*** group joined to a hydrocarbon chain in which all the carbon atoms are linked by ***single bonds***.

The alkanoic acids belong to a wider group of acids known as the carboxylic acids, i.e. any acid which contains the carboxyl group.

There are a number of useful ways of to show the formula of an alkanoic acid, ranging from the full structural formula through various shortened structural formulae to a functional molecular formula (i.e. a type of molecular formula which still has the functional group shown separately). You can see this illustrated for pentanoic acid, the fifth member of the series.

full structural formula:



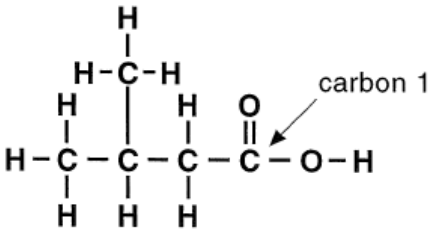
shortened structural formula: $CH_3CH_2CH_2CH_2COOH$

functional molecular formula: $C_4H_9COOH$

The names for alkanoic acids follow the same system that you learned for the alkanes. It is important to make sure that all of the carbon atoms in the main chain are counted. This ***includes the carbon atom in the functional group***. It is easy to forget this carbon, especially when dealing with a functional molecular formula. Thus $\mathbf{C_2H_5COOH}$ has a ***three-carbon*** chain (***not*** two) and is called ***propanoic acid***.

The structure shown is a branched isomer of $C_4H_9COOH$, called ***3-methylbutanoic acid***.

Notice that the main chain is numbered starting with the carbon atom within the functional group as number 1.




Think

Think about the structural formula shown above

- Why is the number in front of methyl '***3***' and not '***2***'?
- Why is ***1-methylbutanoic acid*** not possible as a structure?
- Why is ***4-methylbutanoic acid*** an incorrect name although this structure is possible? (Hint: Draw its structure and consider the correct name.)

What to do

Work out the structural formulae for the following alkanoic acids:

***a)*** *4-methylpentanoic acid* ***b)*** *2-ethylbutanoic acid*

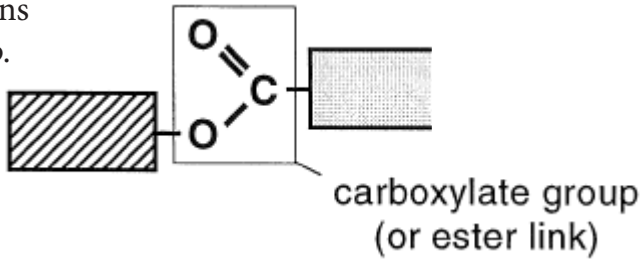
***c)*** *2,2-dimethylpropanoic acid*

Notes

*This activity revises the naming and drawing of full and shortened structural formulae for esters.*

The group of atoms between the two hydrocarbon chains in an ester molecule is known as the ***carboxylate*** group.

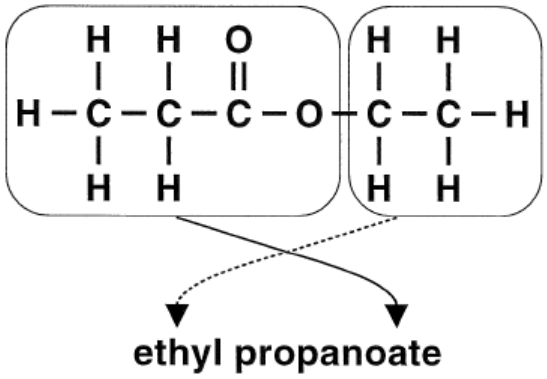
The ***carboxylate*** group is the *functional group* in an ester since this group determines the general chemical properties of all esters. All ester molecules contain the ***carboxylate*** group.




Because the ***carboxylate*** group is the link between two hydrocarbon chains in an ester molecule it is also referred to as the '***ester link***'.

In previous courses, you have seen how the name of an ester is related to its parent alcohol and parent carboxylic acid. You should also be able to name an ester directly from its formula and be able to draw a structural formula directly from the ester name.

**Example**




First find the **C = O** in the carboxylate group. The section of the structure which ***includes*** the carboxylate carbon was part of the ***parent acid*** and gives the ***second*** word of the ester name and ends in '***oate***' .

In this example there are **3** carbon atoms in this section, so the second word in the ester name is ***propanoate***.

The other section of the structure comes from the ***parent alcohol*** gives the first part of the name and ends in '***yl***'. In this example there are **2** carbon atoms in this section, so the first word in this ester name is ***ethyl***.

You will notice that the full structural formula is the opposite way round to the name in this particular example. In fact, ester structures are quite commonly drawn this way round (***parent acid*** first) though you are free to draw it the other way round.

The shortened structural formula for ethyl propanoate can also be written two ways round.

$CH_3CH_2COO\,CH_2CH_3$ or $CH_3CH_2OOCCH_2CH_3$

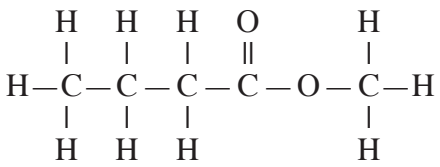
**Think**

Think about the example of ethyl propanoate shown above.

- Which shortened structural formula is the same way round as the full structural formula? How did you decide?
- Which shortened structural formula is the same way round as the ester name? How did you decide?

**What to do**

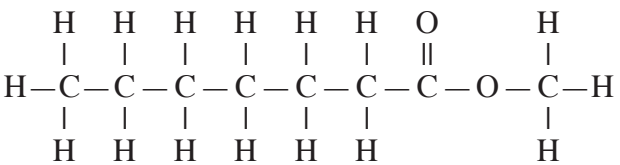
For each of the following, work out the systematic name and/or full structutal formula and/or shortened structural formula as appropriate:



**Notes**

$CH_3CH_2CH_2COOCH_2CH_2CH_2CH_3$

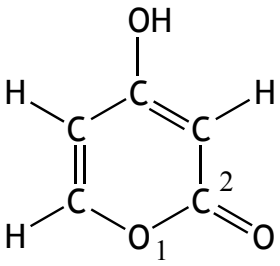
***pentyl propanoate***



# HOME PRACTICE 5.2

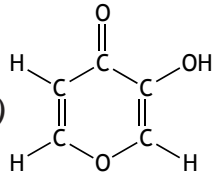
***Q1.*** A Pyrone ring is a hexagonal ring with one corner occupied by an oxygen atom whilst one of the other carbons is a carbonyl group.

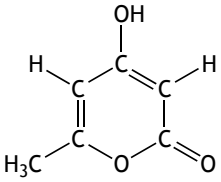
The position of the carbonyl group is identified by a number, counting from the oxygen atom within the ring.

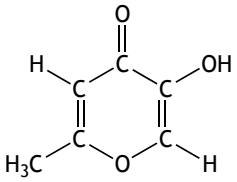


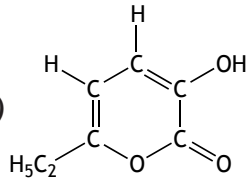
***4-hydroxy-2-pyrone***

Suggest a name for each of the following.

***a)*** 

***b)*** 

***c)*** 

***d)***  **4**

***Q2.*** Shown below are a number of chain and branched alkanols.

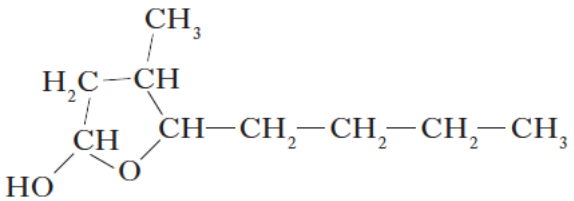
| | |
|---|---|
| A | $CH_3CH_2CH_2CH_2OH$ |
| B | $CH_3CH_2CH(OH)CH_3$ |
| C | $CH_3CH(CH_3)CH_2OH$ |
| D | $CH_3CH_2CH_2CH_2CH_2OH$ |
| E | $CH_3CH_2CH_2CH(OH)CH_3$ |
| F | $CH_3CH_2CH(CH_3)CH_2OH$ |

| | |
|---|---|
| G | $CH_3CH_2C(OH)(CH_3)CH_3$ |
| H | $CH_3CH_2CH_2CH_2CH_2CH_2OH$ |
| I | $CH_3CH_2CH_2CH(CH_3)CH_2OH$ |
| J | $CH_3CH_2CH_2C(OH)(CH_3)CH_3$ |

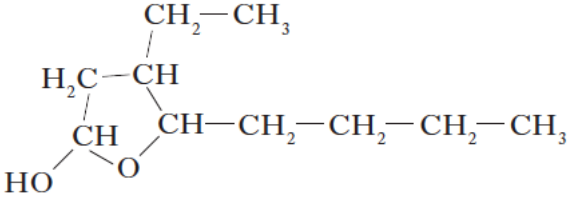
***a)*** Sort them into primary, secondary and tertiary alcohols. **3**

***b)*** Give the systematic names for (C), (G) and (J). **3**

***Q3.*** ***5-Butyl-4-methyltetrahydrofuran-2-ol*** is a flavour compound found in whisky stored in oak barrels.



Write the systematic name for this compound.

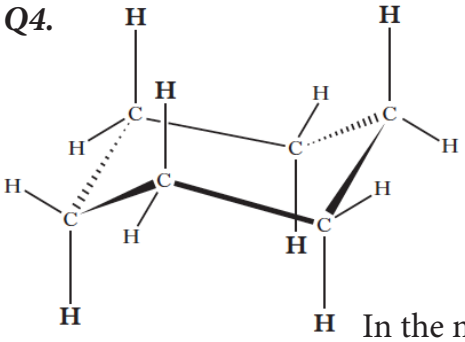


**1**

***Total (11)***

# HOME PRACTICE 5.2

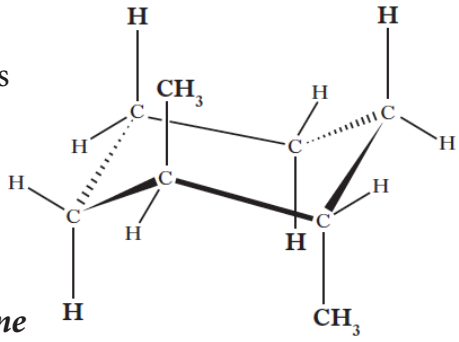
***Q4.***



Cycloalkanes are found in nature.

A representation of cyclohexane is shownon the left.

The six hydrogen atoms marked in **bold** are said to be in axial positions.



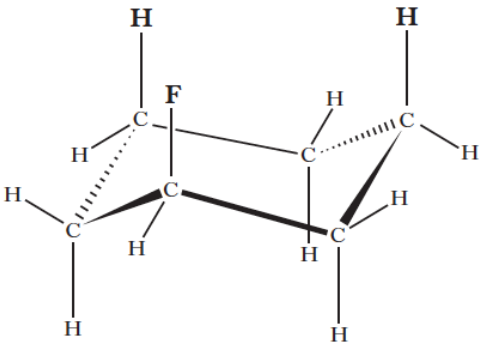
In the molecule of ***1,2-dimethylcyclohexane*** shown on the right, two methyl groups are in axial positions

***a)*** Draw the structure of a molecule of ***1,3-dimethylcyclohexane*** in which both the methyl groups are in axial positions. **1**

***b)*** Axial groups on the same side of a cyclohexane ring can repel each other. The strength of the repulsion is known as the "steric strain".

The table below shows values which allow the steric strain to be calculated.

| Axial groups | Steric strain /kJ mol$^{-1}$ |
|---|---|
| H and H | 0·0 |
| H and F | 0·5 |
| H and Br | 1·0 |
| H and $CH_3$ | 3·8 |
| H and $(CH_3)_3C$ | 11·4 |



For example:

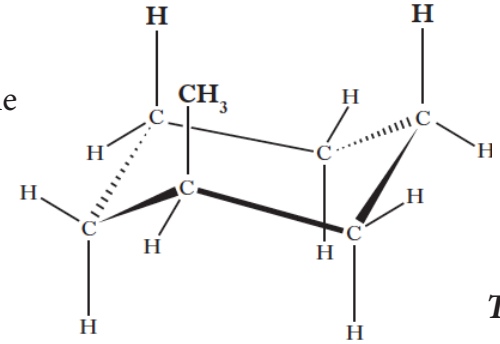
Steric strain = 2 x(Steric strain between **H** and **F**)

= 2 x 0.5

= 1.0 kJ mol$^{-1}$

***i)*** Write a general statement linking the size of steric strain to the type of axial group present. **1**

***ii)*** Calculate, in kJ mol$^{-1}$, the steric strain for the molecule shown opposite.



**1**

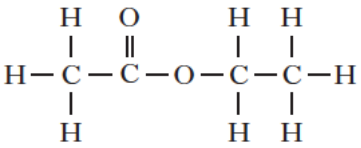
***Total (3)***

# HOME PRACTICE 5.2

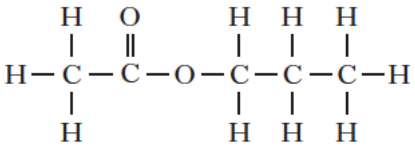
***Q1.*** Hydrolysis of an ester gave an alcohol and a carboxylic acid both of which had the same molecular mass of 60.

***a)*** The structure of the ester was.

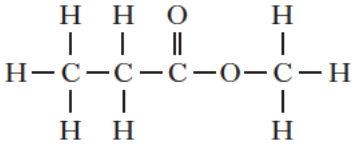
**A**



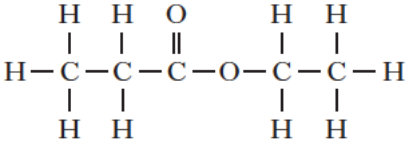
**B**



**C**



**D**

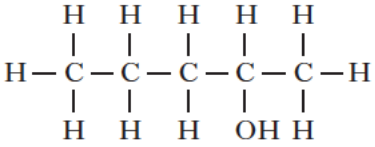


**1**

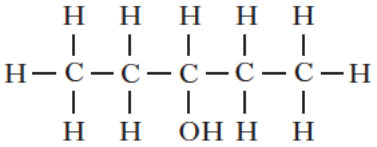
***b)*** Name each ester. **4**

***Q2.*** Shown below are a number of chain and branched alkanols.

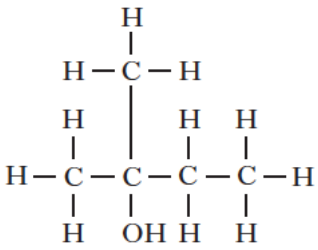
**A**



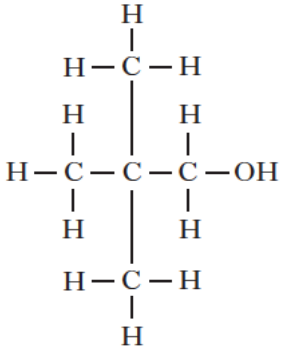
**B**



**C**



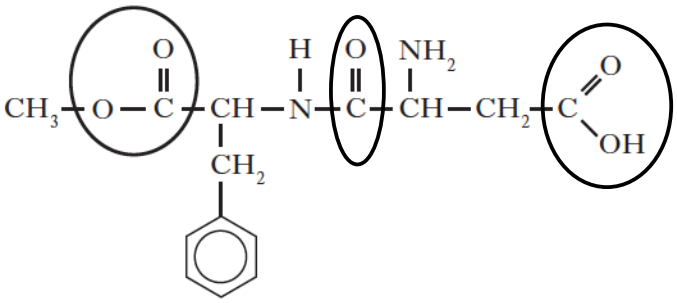
**D**



***a)*** Which alcohol could be oxidised to an alkanal. **1**

***b)*** Give the systematic names for each alkanol . **4**

***Q3.*** Aspartame is added to many soft drinks as a sweetener. Its structure is shown below.



Name all the functional groups circled. **3**

***Total*** ***(13)***