ChemFactsheet

www.curriculum-press.co.uk Number 91

Naming of Organic Compounds

To succeed in this topic you need to understand:
- **the difference between aliphatic and aromatic compounds;**
- **functional groups (covered in Factsheet 15);**
- **homologous series (covered in Factsheet 15);**
- **isomerism (covered in Factsheet 15).**

After working through this Factsheet you will have a more detailed knowledge of organic nomenclature, introduced in Factsheet 15. In particular, you will:
- **understand the systematic naming of alkanes;**
- **understand how other aliphatic compounds are named as substituted alkanes;**
- **know that international (IUPAC) names may differ from those used in UK schools;**
- **know the names of common aromatic compounds.**

Although some organic compounds have trivial names (common names), most of them have to be named systematically. Both the International Union of Pure and Applied Chemistry (IUPAC) and the Association for Science Education (ASE) have published rules of nomenclature, but only ASE names have been adopted by schools in the UK. This Factsheet concentrates on these but also draws your atttention to IUPAC names, where they differ from ASE ones, because you may come across them in your wider reading.

Aliphatic compounds

Alkanes must be studied first, because the names of other aliphatic compounds are based on those of the alkanes.

Alkanes

Remember *- Alkanes are saturated aliphatic hydrocarbons of general formula* C_nH_{2n+2}.

The names of the first ten unbranched alkanes are shown in Table 1.

Table 1 - Names of unbranched alkanes

Formula	Name
CH_4	methane
CH_3CH_3	ethane
$CH_3CH_2CH_3$	propane
$CH_3(CH_2)_2CH_3$	butane
$CH_3(CH_2)_3CH_3$	pentane
$CH_3(CH_2)_4CH_3$	hexane
$CH_3(CH_2)_5CH_3$	heptane
$CH_3(CH_2)_6CH_3$	octane
$CH_3(CH_2)_7CH_3$	nonane
$CH_3(CH_2)_8CH_3$	decane

Branched chain isomers are named as alkyl-substituted alkanes.

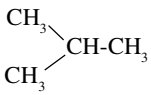
Remember - Isomers are compounds with the same molecular formula but different structural formulae.

An *alkyl* radical (or alkyl group) is derived from an alkane by the loss of one hydrogen atom. The names of alkyl radicals commonly used in organic nomenclature are shown in Table 2.

Table 2 - Names of alkyl radicals

Formula	Name
CH_3-	methyl
CH_3CH_2- or C_2H_5-	ethyl
$CH_3CH_2CH_2$-*	propyl
$CH_3\underset{\vert}{C}HCH_3$	isopropyl (IUPAC) or 1-methylethyl (ASE)

* **Never** write C_3H_7-. This is ambiguous because it could represent either $CH_3CH_2CH_2$- (propyl) or $(CH_3)_2CH$- (isopropyl).

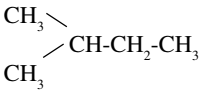


or $(CH_3)_2CHCH_3$ Compound I

In this way, Compound I, commonly called isobutane, is named systematically as methylpropane.

For more complicated molecules, other IUPAC rules are needed.

- Consider Compound II

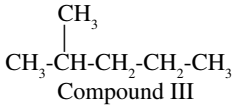


or $(CH_3)_2CHCH_2CH_3$ Compound II

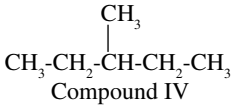
Is this methylbutane or ethylpropane?

For alkanes, always select the longest carbon chain as the basis of the name.

Because the longest chain in Compound II contains four carbon atoms, its correct name is methylbutane. Now consider Compounds III and IV.



Compound III



Compound IV

They both appear to be methylpentane, but two compounds cannot have the same name.

Number the carbon atoms of the longest chain to facilitate reference to substituent groups.

In this way Compound III becomes 2-methylpentane while Compound IV is 3-methylpentane. Numbers used in naming are called *locants*.

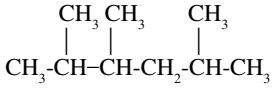
- If the longest chain of Compound III were to be numbered from right to left, the CH_3 group would appear on the fourth carbon atom to give a name of 4-methylpentane rather than 2-methylpentane. Which is right?

In the event of a choice, always select the name with the lower numbering on the occasion of the first difference.

The correct name of Compound III is therefore 2-methylpentane.

Exam Hint *- For complicated molecules you should:*
- *number the C atoms of the longest chain from left to right and write down the name;*
- *number the atoms in the opposite direction and again write down the name;*
- *choose the name with the lower numbering.*

- Look at Compound V.



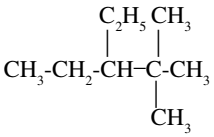
Compound V

On the basis of the rules so far, the name would be 2-methyl-3-methyl-5-methylhexane. This, however, is wrong.

All alkyl groups of a particular kind should be grouped together with a multiplying prefix; di, tri, tetra, penta and hexa for 2, 3, 4, 5 and 6, respectively.

Compound V is therefore 2,3,5-trimethylhexane.

- Finally, consider Compound VI.



Compound VI

Is this called 3-ethyl-4,4-dimethylpentane, or 2,2-dimethyl-3-ethylpentane?

Akyl groups are referred to in alphabetical order.

This rule is applied regardless of any multiplying prefixes. It follows that Compound VI is correctly named as 3-ethyl-4,4-dimethylpentane.

Exam Hint - *It is impossible to have '2-ethyl' anything, except when naming alkenes (see below). If ever you find yourself writing this, it means you've failed to identify the longest carbon chain.*

Alkenes

Remember *- Alkenes are unsaturated aliphatic hydrocarbons with a carbon-carbon double bond. Their general formula is* C_nH_{2n}.

Alkenes are treated as alkanes, with the name ending changed from 'ane' to 'ene', e.g.

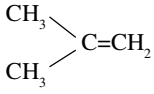
$CH_2=CH_2$ ethene
$CH_3CH=CH_2$ propene

If necessary, locants are used to distinguish between isomers, e.g.

$CH_2=CHCH_2CH_3$ but-1-ene
$CH_3CH=CHCH_3$ but-2-ene

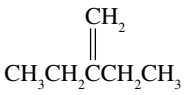
The locant refers to the number of the C atom where the double bond ***starts***.

Branched chain alkenes are named like branched chain alkanes, e.g.



2-methylpropene

The name must always be based on the longest C chain **which includes the C=C bond.** This is not necessarily the same as the longest chain in the molecule. Look at the following compound.



2-ethylbut-1-ene

The longest chain in this molecule has five C atoms, but the compound cannot be named as a derivative of pentane because there is no way of referring to the $=CH_2$ side chain.

Dienes, i.e. compounds with two C=C bonds, are named as such. There must be a locant to denote the position of each double bond, e.g.

$CH_2=CHCH=CH_2$ buta-1,3-diene

Variations

The trivial names ethylene (for C_2H_4) and propylene (for C_3H_6) are in common use. IUPAC places locants at the beginnings of names rather than within them, e.g.

$CH_2=CHCH_2CH_3$ 1-butene
$CH_3CH=CHCH_3$ 2-butene

Haloalkanes or **halogenoalkanes** (Formerly known as alkyl halides)

Remember - These are compounds of the kind RX, where R stands for an alkyl radical, such as CH_3 *or* C_2H_5*, and X for a halogen atom; Cl, Br or I.*

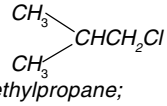
Haloalkanes are given *substitutive names*, i.e. they are named as halogen-substituted alkanes.

Write down 'chloro', 'bromo' or 'iodo', followed by the name of the parent alkane.

Use locants, if necessary, to indicate the positions of both alkyl groups and the halogen atom, e.g.

CH_3Cl chloromethane
CH_3CH_2Br bromoethane
$CH_3CH_2CH_2I$ 1-iodopropane
CH_3CHICH_3 2-iodopropane

Exam Hint - *Beware of the following compound:*



This is called 1-chloro-2-methylpropane;
NOT 2-methyl-1-chloropropane.
In all haloalkanes, the 'halo' part of the name comes first.

Variations

As well as substitutive names, IUPAC also allows *radicofunctional names*. On this system, the compounds are named as alkyl halides, e.g.

CH_3Cl methyl chloride
CH_3CH_2Br ethyl bromide
$CH_3CH_2CH_2I$ n-propyl iodide*
CH_3CHICH_3 isopropyl iodide

* n stands for 'normal'.

Alcohols

Remember *- Alcohols are compounds of the kind ROH, where R represents an alkyl radical and OH (hydroxyl) is the functional group.*

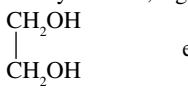
Alcohols are named as alkanols, i.e. they are treated as hydroxyl-substituted alkanes.

Write down the name of the parent alkane, delete 'e' from the end and replace it by 'ol'.

Use locants where necessary to refer to the positions of both alkyl side chains and the OH group, e.g.

CH_3OH	methanol
CH_3CH_2OH	ethanol
$CH_3CH_2CH_2OH$	propan-1-ol
$CH_3CH(OH)CH_3$	propan-2-ol
$CH_3CH_2CH_2CH_2OH$	butan-1-ol
$CH_3CH(OH)CH_2CH_3$	butan-2-ol
$(CH_3)_2CHCH_2OH$	2-methylpropan-1-ol
$(CH_3)_3COH$	2-methylpropan-2-ol

Dihydric alcohols (compounds with two OH groups) are named systematically as diols, e.g.



ethane-1,2-diol

The trivial name of this compound is ethylene glycol.

Variations

IUPAC substitutive names differ from ASE ones in that the locant is written at the beginning of the name, e.g. 1-propanol instead of propan-1-ol. IUPAC also allows the use of radicofunctional names, e.g.

CH_3OH	methyl alcohol
CH_3CH_2OH	ethyl alcohol
$CH_3CH_2CH_2OH$	n-propyl alcohol
$CH_3CH(OH)CH_3$	isopropyl alcohol

The chemical industry uses some hybrid names, notably the following:

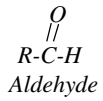
$CH_3CH_2CH_2OH$	n-propanol
$CH_3CH(OH)CH_3$	isopropanol
$CH_3CH_2CH_2CH_2OH$	n-butanol
$CH_3CH(OH)CH_2CH_3$	sec-butanol
$(CH_3)_2CHCH_2OH$	isobutanol
$(CH_3)_3COH$	tert-butanol

Aldehydes and ketones

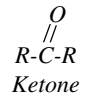
Remember

Aldehydes and ketones all contain the carbonyl group, 

The difference between them is that, in an aldehyde molecule, at least one bond from the carbonyl carbon atom is joined to H whereas, in the case of a ketone, both bonds are joined to alkyl radicals.



Aldehyde



Ketone

Aldehydes are named as alkanals and ketones as alkanones.

Aldehydes *Write down the name of the parent alkane, delete 'e' from the end and replace it by 'al'.*

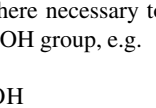
Ketones *Write down the name of the parent alkane, delete 'e' from the end and replace it by 'one'.*

For aldehydes, it is unnecessary to use a locant to show the position of the C=O group because it is always situated at the end of the chain:

HCHO	methanal
CH_3CHO	ethanal
CH_3CH_2CHO	propanal
$CH_3CH_2CH_2CHO$	butanal

Exam Hint - *Always write the formula of an aldehyde as RCHO; not RCOH, because this implies the presence of a hydroxyl group.*

When naming branched chain aldehydes, it is assumed that the C atom of CHO is no. 1 of the longest chain, e.g.



3-methylbutanal

For ketones, a locant is generally needed for the C atom of the CO group, e.g.

CH_3COCH_3	propanone
$CH_3COCH_2CH_3$	butan-2-one
$CH_3COCH_2CH_2CH_3$	pentan-2-one
$CH_3CH_2COCH_2CH_3$	pentan-3-one
$(CH_3)_2CHCOCH_3$	3-methylbutan-2-one

Variations

For aldehydes, IUPAC permits a series of older names based on the trivial names of the carboxylic acids to which they become oxidised, e.g.

HCHO	formaldehyde
CH_3CHO	acetaldehyde
CH_3CH_2CHO	propionaldehyde

For the substitutive names of ketones, IUPAC recommends that the locant should be placed at the beginning of the word, e.g. 2-pentanone instead of pentan-2-one. IUPAC also allows radicofunctional names, e.g. ethyl methyl ketone for $CH_3COCH_2CH_3$.

For the first member of the homologous series, CH_3COCH_3, the trivial name of acetone is still widely used, especially in industry.

Carboxylic acids

Remember *- Carboxylic acids are compounds of the kind RCOOH. The functional group, COOH, is called the carboxyl group.*

These compounds are named systematically as alkanoic acids.

Write down the name of the parent alkane, delete 'e' from the end and replace it by 'oic acid'.

As for aldehydes, a locant is not needed to show the position of the functional group. The C atom of the COOH group is assumed to be C atom no. 1 of the longest chain, e.g.

HCOOH	methanoic acid
CH_3COOH	ethanoic acid
CH_3CH_2COOH	propanoic acid
$CH_3CH_2CH_2COOH$	butanoic acid
$(CH_3)_2CHCOOH$	2-methylpropanoic acid

Dicarboxylic acids are named as alkanedioic acids, e.g.

ethanedioic acid

Variations

IUPAC recommends retention of trivial names for simple aliphatic acids. These reflect the original sources of the compounds, e.g.

HCOOH	formic acid (from the Latin *formica* = an ant)
CH_3COOH	acetic acid (from the Latin *acetum* = vinegar)
CH_3CH_2COOH	propionic acid (from the Greek *pion* = fat)
$CH_3CH_2CH_2COOH$	butyric acid (from the Latin *butyrum* = butter)

Derivatives of carboxylic acids

Acyl chlorides (Formerly known as acid chlorides)

Remember - These are compounds of the kind RCOCl, i.e. they are derived from carboxylic acids by replacing OH by Cl. A group of the kind RCO is known as an acyl group.

Acyl chlorides (and other acyl halides) are given substitutive names.

Write down the name of the parent alkane, delete 'e' from the end and replace it by 'oyl chloride'.

Effectively, the first member of the homologous series is CH_3COCl, ethanoyl chloride. (HCOCl is an unstable compound: it decomposes into HCl + CO.)

Variations

IUPAC permits radicofunctional names based on the trivial names of the carboxylic acids from which they are derived, e.g.

CH_3COCl acetyl chloride

Esters

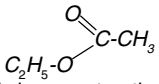
Remember - Esters are of the kind RCOOR', i.e. they are derived from carboxylic acids by replacing H of the carboxyl group by a hydrocarbon radical R'. (R and R' may be identical radicals.

Although esters are generally prepared by reacting carboxylic acids with alcohols, for naming purposes they are regarded as derivatives of carboxylic acids. Thus, all esters of ethanoic acid are called ethanoates, e.g.

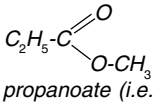
$CH_3COOC_2H_5$ ethyl ethanoate

A IUPAC variation is ethyl acetate.

Exam Hint - *Be very careful how you write the formulae of esters: a wrongly written formula leads to a wrong name. For instance, the formula of ethyl ethanoate could be written $C_2H_5OCOCH_3$, which is a contraction of*



but NOT $C_2H_5COOCH_3$, which is a contraction of



This is the formula of methyl propanoate (i.e. the methyl ester of propanoic acid), a different - although isomeric - ester.

Amides

Remember - Amides have the general formula $RCONH_2$. They are derived from carboxylic acids by replacing OH by NH_2.

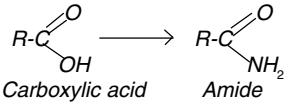
They are given substitutive names.

Write down the formula of the parent alkane, delete 'e' from the end and replace it by 'amide'.

E.g. CH_3CONH_2 ethanamide

A IUPAC alternative is acetamide.

Exam Hint *- Do not confuse amides with amines!*
Amides are derived from carboxylic acids:



Carboxylic acid *Amide*

Amines (see below) are derived from alcohols:

R-OH ⟶ *R-NH_2*

Alcohol *Amine*

If in doubt, refer to amides as 'acid amides'. This is an old-fashioned term but it might help.

Amides in which H atoms of the NH_2 group are replaced by alkyl radicals are named as *N*-substituted amides, i.e. nitrogen-substituted amides, e.g.

$CH_3CONHC_2H_5$ *N*-ethylethanamide

(The formula could equally well be written as $C_2H_5NHCOCH_3$, but ***not*** $C_2H_5CONHCH_3$ because this represents *N*-methylpropanamide.)

Nitriles

Remember *- Nitriles are organic cyanides; compounds of the kind RCN.*

These compounds are given substitutive names, formed by adding the suffix 'nitrile' to the name of the parent alkane, e.g.

CH_3CN ethanenitrile

IUPAC also allows radicofunctional names, such as methyl cyanide for CH_3CN.

Exam Hint - *When looking for the longest carbon chain in a nitrile molecule, don't forget to include the C atom of the CN group!*

Amines

Remember *- Aliphatic amines are alkyl derivatives of ammonia.*

Ammonia *Primary amine* *Secondary amine* *Tertiary amine*

Only primary amines are included in current A-level specifications. Both ASE and IUPAC recommend the retention of radicofunctional names rather than the adoption of substitutive ones. Any differences between the two systems are due to variations in the names of hydrocarbon radicals, e.g.

CH_3NH_2	methylamine (not 'aminomethane')
$CH_3CH_2NH_2$	ethylamine
$CH_3CH_2CH_2NH_2$	propylamine
$CH_3CH(NH_2)CH_3$	(1-methylethyl)amine - ASE or isopropylamine - IUPAC

Difunctional aliphatic compounds

If a molecule contains two functional groups, one of which is represented by a prefix and the other by a suffix, there is no difficulty with naming, e.g.

$CH_3CHClCOOH$ 2-chloropropanoic acid

Life, however, is not always that straightforward!

*If **both** functional groups are normally represented by suffixes, there is a problem which is overcome by citing the principal one as a suffix and the other as a prefix.*

Prefixes in common use include the following:

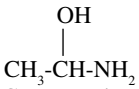
hydroxy for OH
amino for NH_2
keto for CO

The question as to which of two groups is the principal one, for citing as the suffix, can be resolved only by referring to the IUPAC order of priority. An abridged list is provided below.

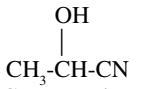
Decreasing priority ↓

-COOH (carboxylic acid)
-CN (nitrile)
-CHO (aldehyde)
>C=O (ketone)
-OH (alcohol)
$-NH_2$ (amine)

Look at the two difunctional compounds VII and VIII, both of which contain an OH group.



Compound VII



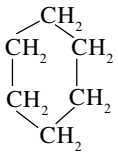
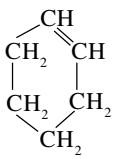
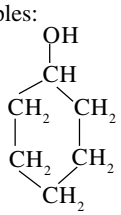
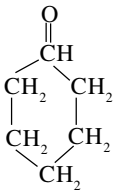
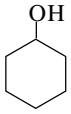
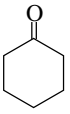
Compound VIII

OH has a higher priority than NH_2, but a lower priority than CN. It is therefore the principal group in Compound VII, and consequently cited as the suffix, but not in Compound VIII, where it is denoted by the prefix hydroxy. Compound VII is named 1-aminoethanol, and Compound VIII is 2-hydroxypropanenitrile.

Alicyclic compounds

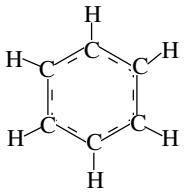
***Remember** - Alicyclic compounds are aliphatic compounds with a ring structure.*

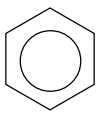
These compounds are named in the same way as aliphatic ones, but with the prefix 'cyclo'. The commonest ones, with a six-membered ring, comprise cyclohexane and its derivatives. Examples:

structural formula				
symbol				
name	cyclohexane	cyclohexene	cyclohexanol	cyclohexanone

Aromatic compounds

The parent compound is benzene, C_6H_6.

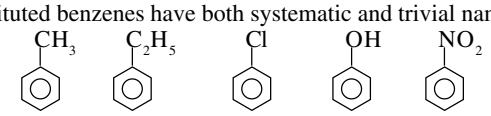

structural formula of bemzene


symbol

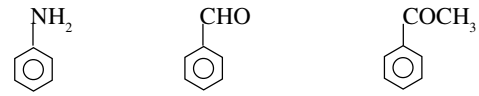
***Exam Hint -** When writing the symbol for benzene, don't forget to include the circle to represent the delocalised π-bond. If you leave it out, and draw only a hexagon, you are writing the formula of cyclohexane.*

Other aromatic compounds are those whose molecules contain at least one benzene ring. (Strictly, an aromatic compound is one whose molecules have a ring structure with a set of six π-electrons, but this definition is not required at A-level.)

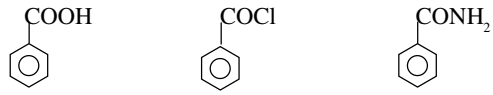
Many monosubstituted benzenes have both systematic and trivial names:



Systematic name:	methyl-benzene	ethyl-benzene	chloro-benzene	-	nitro-benzene
Trivial name:	toluene	-	-	phenol	-



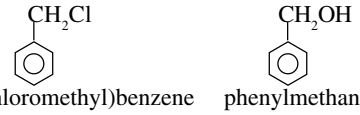
Systematic name:	phenylamine	benzenecarbaldehyde	phenylethanone
Trivial name:	aniline	benzaldehyde	acetophenone



Systematic name:	benzenecarboxylic acid	benzenecarbonyl chloride	benzenecarboxamide
Trivial name:	benzoic acid	benzoyl chloride	benzamide

*Although trivial names are widely used in the chemical industry, only systematic ones are used in schools in the UK. **The only trivial name that is permitted is phenol for C_6H_5OH.***

Some compounds have both substitutive and radicofunctional systematic names, e.g.



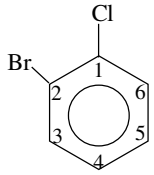
Substitutive name:	(chloromethyl)benzene	phenylmethanol
Radicofunctional name:	benzyl chloride	benzyl alcohol

For aromatic compounds, as for aliphatic ones, UK schools prefer to use substitutive names.

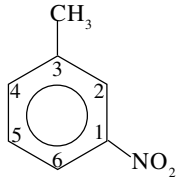
When naming disubstituted and polysubstituted benzenes, a reference group has to be chosen as the basis of the name.

The later group alphabetically is used as a reference, from which position the carbon atoms of the ring are numbered from 1 to 6. This provides locants for denoting the positions of other groups.

Consider Compounds IX and X.



Compound IX



Compound X

For Compound IX, the reference group is Cl because C (for chloro) is later in the alphabet than B (for bromo). The ring is numbered as shown, to give a name of 2-bromochlorobenzene; ***not*** 6-bromochlorobenzene.

For aromatic compounds, as for aliphatic ones, numbers in names should be kept as low as possible.

By similar reasoning, Compound X is regarded as a derivative of nitrobenzene, rather than methylbenzene, so the correct name is 3-methylnitrobenzene.

Practice questions

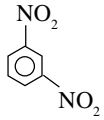
1 Write down the structural formulae of five isomeric compounds of molecular formula C_6H_{14} and name them on the IUPAC system.

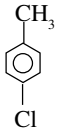
2 Give the systematic name of each of the following compounds.

(a) $(CH_3)_2CHCH_2OH$

(b) $CH_3C(=CH_2)CH_2CH_2CH_3$

(c) $CH_3CH(OH)CH_2CHO$

(d) 

(e) 

3 Write down the structural formula of each of the following compounds.

(a) 2-chloroethanol

(b) propane-1,2,3-triol

(c) 2-methylpent-3-enoic acid

(d) phenylethene

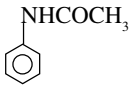
(e) benzenecarboxamide

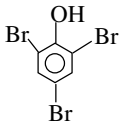
4 Identify which of the following names is/are wrong and then write down the correct systematic name in each case.

(a) $CH_3CH(OH)COOH$ 2-hydroxypropanoic acid

(b) $(CH_3)_3COH$ 2,2-dimethylethanol

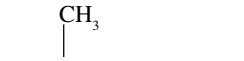
(c)  aminobenzene

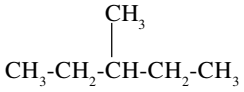
(d)  *N*-phenylethanamide

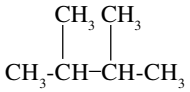
(e)  2,4,6-tribromohydroxybenzene

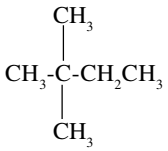
Answers

1 CH_3-CH_2-CH_2CH_2-CH_2-CH_3 hexane

 2-methylpentane

 3-methylpentane

 2,3-dimethylbutane

 2,2-dimethylbutane

2 (a) 2-methylpropan-1-ol

(b) 2-methylpent-1-ene

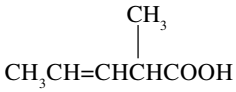
(c) 3-hydroxybutanal

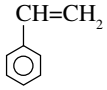
(d) 1,3-dinitrobenzene

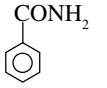
(e) 1-chloro-4-methylbenzene

3 (a) CH_2ClCH_2OH

(b) $CH_2OHCH(OH)CH_2OH$

(c) 

(d)  or $C_6H_5CH=CH_2$

(e)  or $C_6H_5CONH_2$

4 (a) Correct

(b) Wrong Correct name is 2-methylpropan-2-ol

(c) Wrong Correct name is phenylamine

(d) Correct

(e) Wrong Correct name is 2,4,6-tribromophenol

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