Chem Factsheet

www.curriculum-press.co.uk Number 237

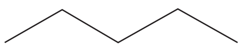
Skeletal Formulae

Organic chemistry requires the use of a range of different types of formulae. Empirical and molecular formulae provide basic information on the numbers of atoms in any given molecule. Structural, displayed and skeletal formulae give information on the arrangement of atoms, especially to any functional groups present. Skeletal formulae are particularly useful in providing a simple representation of larger and more complex organic molecules.

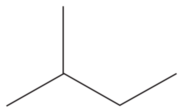
> Skeletal formulae are a simplified means of representing organic compounds that show the carbon skeleton and any functional groups present **only**.

When drawing skeletal formulae all carbon and hydrogen labels are removed, as are any bonds to hydrogen atoms. To emphasise the carbon junctions in the carbon chain, a 'zig-zag' pattern is used, see Fig.1.

Fig. 1



Skeletal formula of pentane, $CH_3CH_2CH_2CH_2CH_3$

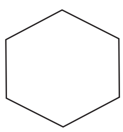


Skeletal formula of 2-methylbutane, $CH_3CH(CH_3)CH_2CH_3$

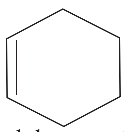
> - Each line represents a single bond
> - A junction or an intersection represents a carbon atom
> - The end of a line represents a $–CH_3$ group

Cyclic compounds are also concisely drawn. Figure 2(a) compares the skeletal formula of cyclohexane and cyclohexene, and Figure 2(b) shows alternative skeletal representations of benzene.

Fig. 2

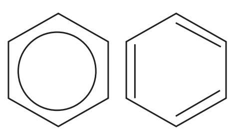


cyclohexane, C_6H_{12}



cyclohexene, C_6H_{10}

(a) Examples of skeletal formulae of cyclic hydrocarbons

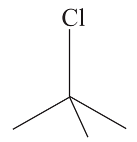


(b) Alternative skeletal representations of benzene, C_6H_6.

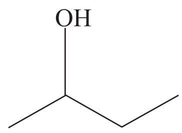
Skeletal formulae representing molecules with functional groups

Functional groups must be included in skeletal formulae and care is taken to represent the type and position of the functional group on the skeletal framework. Figure 3 provides examples of skeletal formulae containing some commonly found functional groups.

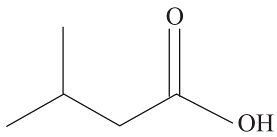
Fig. 3



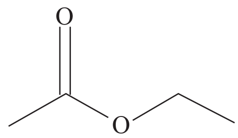
(a) 2-chloro-2-methylpropane $CH_3CCl(CH_3)CH_3$



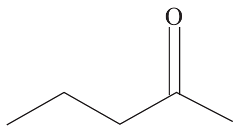
(b) butan-2-ol $CH_3CH(OH)CH_2CH_3$



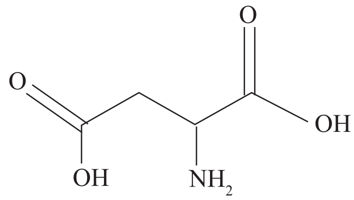
(c) 3-methylbutanoic acid $CH_3CH(CH_3)CH_2COOH$



(d) ethyl ethanoate $CH_3COOCH_2CH_3$



(e) pentan-2-one $CH_3CH_2CH_2COCH_3$



(f) aspartic acid $HOOCCH_2CH(NH_2)COOH$

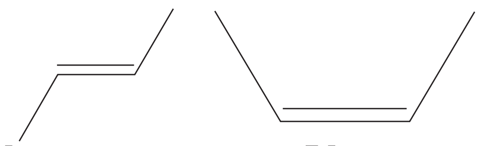
> It is important to connect the bonding skeletal carbon to the correct bonding atom on the functional group. Note in Figure 3(b), the skeletal chain is drawn connected to the oxygen atom of the hydroxyl group, not to the H or "in between" O and H.

Skeletal formulae and stereoisomerism

Stereoisomerism occurs when compounds with the same structural formula have a different arrangement of their atoms in space. It is important when drawing skeletal formulae that different stereoisomers are correctly identified.

E/Z isomers only occur about a carbon-carbon double bond, due to the restriction in rotation allowed by the double bond and the planar shape. The alternative positions of atoms and groups attached to the double bond are therefore fixed. This is simply represented using skeletal formulae with the relative positions of the attached groups easily identified. In the example provided, see Figure 4, the relative positions of the alkyl groups linked to the carbon-carbon double bond is clearly shown. There are two possible stereoisomers; (E) with the alkyl groups aligned on opposite sides of the double bond, and (Z) with the alkyl groups positioned on the same side of the double bond.

Fig. 4

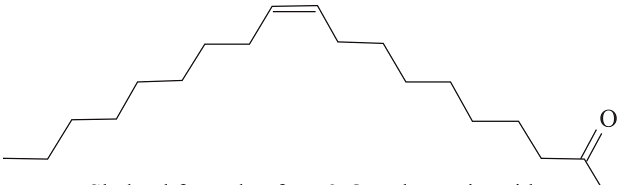


E-Isomer Z-Isomer

Stereoisomers of but-2-ene, C_4H_8

Cis-trans isomerism is used to describe a specific form of E/Z isomerism, where one of the attached groups on each carbon atom on the double bond is a hydrogen atom. This is commonly used in the description of oils and fatty acids. Figure 5 shows the skeletal structure of oleic acid or *cis*-9-octadecenoic acid. (The IUPAC name is (9*Z*)-octadec-9-enoic acid).

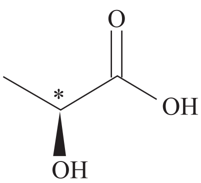
Fig. 5



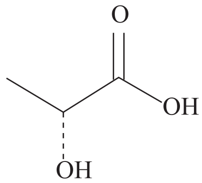
Skeletal formula of *cis*-9-Octadecenoic acid

Optical stereoisomerism occurs when a molecule contains a chiral centre. This is, a carbon atom attached to four different atoms or groups. This gives two stereoisomers (or enantiomers), which are mirror images of each other. They are non-superimposable. The relative positioning around the chiral carbon is achieved using the 'wedge-dash' notation. Figure 6 describes the two enantiomers of lactic acid. Note that the asterisk (*) denotes the chiral centre.

Fig. 6



(a) Skeletal formula for L-Lactic Acid $CH_3CH(OH)COOH$



(b) Skeletal formula for D-Lactic Acid $CH_3CH(OH)COOH$

The hydrogen atom on the chiral carbon is not drawn as part of the skeletal formula. However, this example illustrates how the hydrogen atom bonded to the chiral centre is still taken into account as one of the four different groups attached to the central carbon atom.

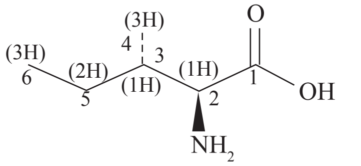
Examination examples

Skeletal formulae are often used in text books and examination questions. It is therefore important to be able to understand and interpret the use of skeletal formulae.

> Read examination questions carefully as they will often specify the type of formula required. Marks will be lost if the type of formula used in the answer is not the one asked for, even if the formula itself is correct.

> When asked to obtain a molecular formula from a skeletal formula, avoid miscounting the number of carbon and hydrogen atoms by 'adding' them to the skeletal formula provided in the question. See Figure 7.

Fig. 7



Molecular Formula $C_6H_{13}NO_2$

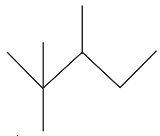
2–amino–3–methylpentanoic acid (isoleucine)

Questions

1. Draw the skeletal formulae of the following molecules:
   (a) 2,3–dimethylbutane
   (b) 3–methylbutan–1–ol
   (c) pentanoic acid
   (d) (E) 3–methylheptene–3–ene
   (e) 3–hydroxybutanal
   (f) 2–phenylpropane
   (g) butan–2–ol (giving both enantiomers)

2. For each of the following skeletal formulae; give the correct molecular formula, and name the molecule.

(a)



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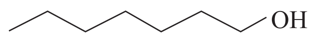
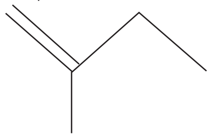
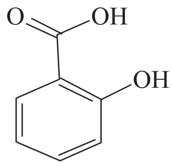


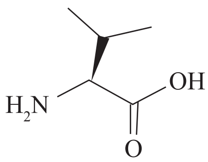
(c)



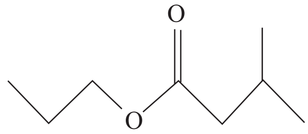
(d)



(e)



(f)

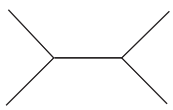


3. Review your answers to Question 2 and identify any chiral centres that are present. Label each chiral carbon in the skeletal formulae with an asterisk (*).

4. Vaccenic acid is a naturally occurring trans-fatty acid found in dairy products. Its IUPAC name is (*E*)-octadec-11-enoic acid. Draw the skeletal formula of trans–vaccenic acid.

Answers

1. (a)



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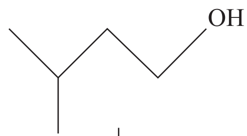

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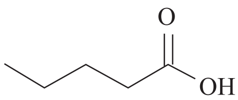

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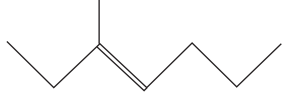
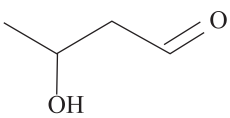
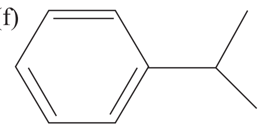


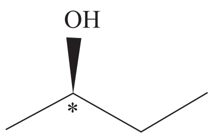
(e)

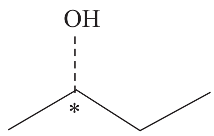


(f)



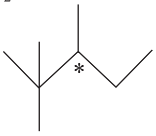
(g)



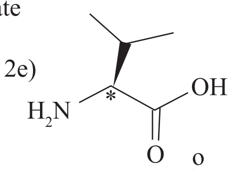


2. (a) C_8H_{18} 2,2,3–trimethypentane (b) $C_7H_{16}O$ heptan–1–ol
   (c) C_5H_{10} 2–methylbut–1–ene (d) $C_7H_6O_3$ 2–hydroxybenzoic acid
   (e) $C_5H_{11}NO_2$ 2–amino–3–methylbutanoic acid
   (f) $C_8H_{16}O_2$ propyl–3–methylbutanoate

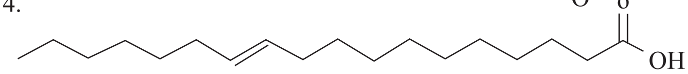
3. See 2a)



See 2e)



4.



Acknowledgements: This Factsheet was researched and written by Gareth Riley ***ISSN 1351-5136***