

# 9

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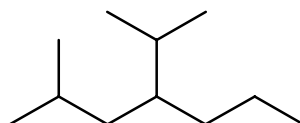
## The language of organic chemistry

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### Answers to worked examples

#### WE 9.1 Naming alkanes (on p. 419 in *Chemistry*<sup>3</sup>)

Give the IUPAC name of the following compound.

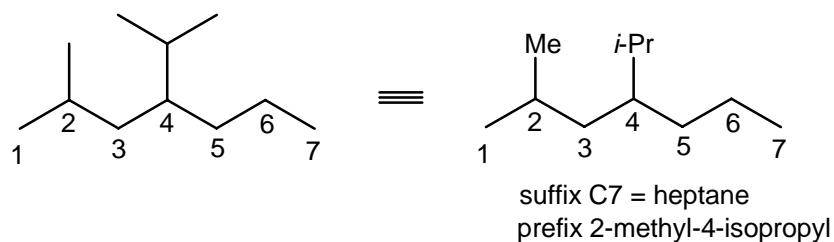


#### Strategy

1. Identify the longest continuous carbon chain. All alkane names end with –ane.
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

#### Solution

1. The longest continuous carbon chain has SEVEN carbon atoms; and therefore its suffix is heptane.
2. For this molecule, the carbon atoms are numbered from left to right as 4-isopropyl-2-methyl has lower numbers than 4-isopropyl-6-methyl. [Remember: isopropyl comes before methyl, as **i** is before **m** in the alphabet.]
3. The name of this compound is 4-isopropyl-2-methylheptane.



Answer

4-Isopropyl-2-methylheptane

**WE 9.3 Naming alkenes (on p. 423 in *Chemistry*<sup>3</sup>)**

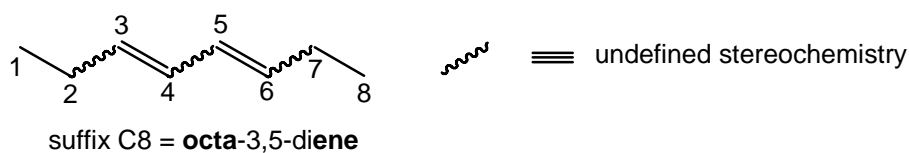
Draw the *cis*-, *cis*- and *cis*-, *trans*- isomers of octa-3,5-diene.

Strategy

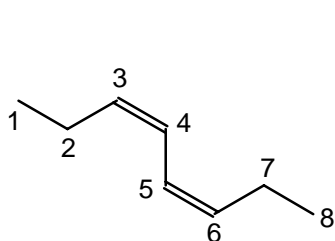
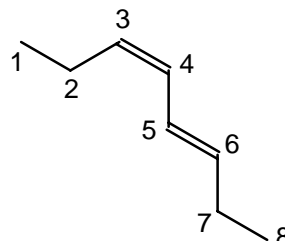
1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
  2. Draw out the double bonds at their designated positions.
  3. A *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond. A diene contains two C=C bonds.
  4. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
1. Check that this structure is correct!

Solution

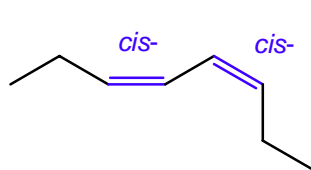
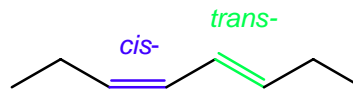
1. The longest number of continuous carbon atoms is eight (**octa-3,5-diene**). Draw out this carbon chain for both isomers.
2. The suffix of this molecule is ene (**octa-3,5-diene**); it is therefore an alkene. This molecule contains two double bonds (**octa-3,5-diene**), and they are positioned at carbons **3** ( $\rightarrow$ 4) and **5** ( $\rightarrow$ 6).



3. The *cis*, *cis*-isomer is where both double bonds at carbons **3** ( $\rightarrow$ 4) and **5** ( $\rightarrow$ 6) have their substituents on the *same side* of the double bond. For the stereoisomeric *cis*-, *trans*-isomer, the double bonds at carbons **3** ( $\rightarrow$ 4) and **5** ( $\rightarrow$ 6) have *cis*- and *trans*-configurations, respectively. A *trans*-isomer is where the substituents are on *opposite sides* of the double bond. A diene contains two C=C bonds.

*cis*-,*cis*-octa-3,5-diene*cis*-,*trans*-octa-3,5-diene

4. There are no additional substituents.  
5. Check that these structures are correct by re-naming it! This structure is 4-*tert*-butyl-3,3-dimethylheptane.

Answer*cis*-,*cis*-octa-3,5-diene*cis*-,*trans*-octa-3,5-diene**WE 9.5 Naming halogenoalkenes (on p. 427 in *Chemistry*<sup>3</sup>)**

Draw the skeletal structure of 5,6-dichloro-2-methyloct-2-ene. Are the chlorine atoms bonded to primary, secondary, or tertiary carbon atoms?

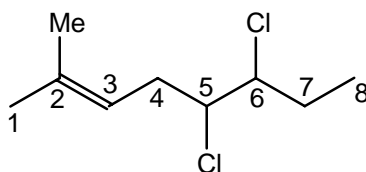
Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Draw out the double bond at its designated position.
3. If stereochemistry is present; a *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.

- Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
- Check that this structure is correct!

Solution

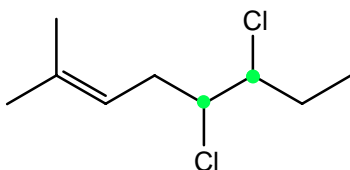
- The longest number of continuous carbon atoms is eight (**oct-2-ene**). Draw out this carbon chain.
- The suffix of this molecule is ene (**oct-2-ene**); it is therefore an alkene. This molecule contains a single double bond (**oct-2-ene**), and this is positioned at carbons **2 to 3** (2→3).
- There is no stereochemistry present.
- There are two different substituents; a methyl (Me-) group at carbon-2, and two chloro-substituents at carbons-5 and 6.



suffix C8 = **oct-2-ene**  
 prefix **5,6-dichloro-2-methyl**

- Check that this structure is correct by re-naming it! This structure is 5,6-dichloro-2-methyloct-2-ene.

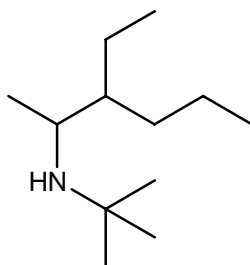
Answer



● = secondary carbon atom  
 5,6-dichloro-2-methyloct-2-ene

**WE 9.7 Naming and classifying amines (on p. 432 in *Chemistry*<sup>3</sup>)**

Give the IUPAC name of the following amine and classify the amine as primary, secondary, or tertiary.

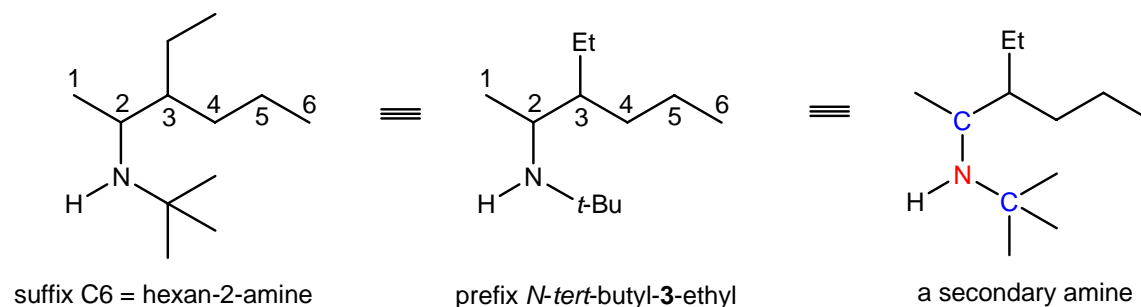


### Strategy

1. Identify the longest continuous carbon chain and remember to number the carbon atoms so that the amine group has the lowest possible number.
2. Identify the two remaining groups attached to the nitrogen atom of this amine; this name is preceded by *N,N*- (which states that these substituents are attached to this nitrogen atom).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.
4. Count the number of alkyl groups attached to this nitrogen atom to determine if this amine is primary ( $1^\circ$ ), secondary ( $2^\circ$ ) or tertiary ( $3^\circ$ ).

### Solution

1. The longest continuous carbon chain has SIX carbon atoms; and therefore its suffix is **hexane**. For this alkanamine, the (lowest possible number for this) amine group is on carbon-2.
2. The two remaining groups attached to this nitrogen atom are *tert*-butyl and hydrogen. This amine is *N-tert*-butyl amine.
3. There is one remaining substituent, an ethyl (Et) group at carbon-3. This amine is 3-ethylhexan-2-amine. Its overall name is *N-tert*-butyl-3-ethylhexan-2-amine.



4. This amine is a secondary amine as the (red) nitrogen atom has TWO (blue) alkyl groups attached to it. The name of this compound is *N-tert-butyl-3-ethylhexan-2-amine*.

Answer

*N-tert-butyl-3-ethylhexan-2-amine*. This is a secondary amine.

**WE 9.9 Drawing and naming esters (on p. 440 in *Chemistry*<sup>3</sup>)**

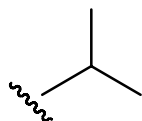
Draw the skeletal structure of isopropyl benzoate.

Strategy

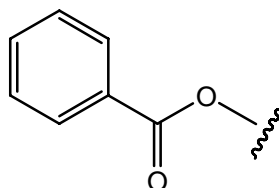
1. This molecule is an isopropyl ester. The parent carboxylate is benzoate. Draw out the carbon skeleton of these components.
2. Check that the structure you have drawn is correct!

Solution

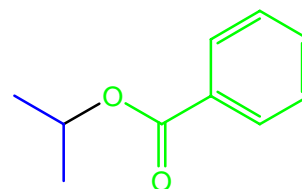
1. An isopropyl group is  $\text{Me}_2\text{CH}-$ , and a benzoate group is  $\text{PhCO}_2-$ . By connecting these two fragments together reveals the structure of the required ester.



an isopropyl group



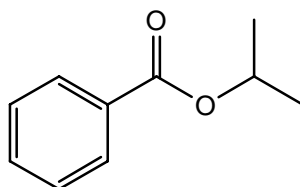
a benzoate group



isopropyl benzoate

2. Check that this structure is correct by re-naming it! This structure is isopropyl benzoate.

Answer



isopropyl benzoate

## Answers to boxes

### Box 9.5 The DDT dilemma (on p. 428 in *Chemistry*<sup>3</sup>)

Some insects have developed a resistance to DDT by producing enzymes that catalyse the conversion of DDT into a related compound called 1,1-dichloro-2,2-di(4-chlorophenyl)ethene (DDE). DDE is not an insecticide as this compound is flatter than DDT and the change in shape alters the toxicity.

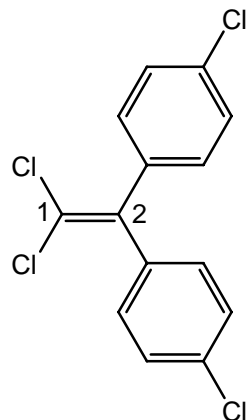
Draw the skeletal structure for DDE.

#### Strategy

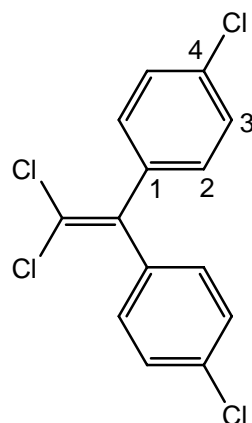
1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Draw out the double bond at its designated positions.
3. If stereochemistry is present; a *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.
4. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
5. Check that this structure is correct!

#### Solution

1. The longest number of continuous carbon atoms is two (**ethene**). Draw out this carbon chain.
2. The suffix of this molecule is ene (**ethene**); it is therefore an alkene. This molecule contains a single double bond, and this is positioned at carbon **1** ( $\rightarrow$ 2).
3. There is no stereochemistry present.
4. There are two different substituents; two chloro- (Cl-) substituents at carbon-1, and two 4-chlorophenyl- (4-ClC<sub>6</sub>H<sub>4</sub>-) groups at carbon-2.



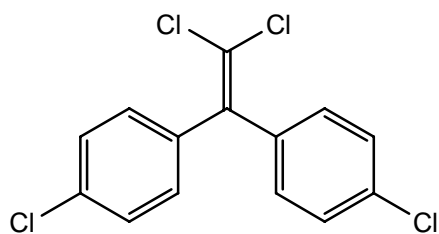
suffix C2 = ethene



prefix 1,1-dichloro-2,2-di(4-chlorophenyl)

5. Check that this structure is correct by naming it! This structure is 1,1-dichloro-2,2-di(4-chlorophenyl)ethene.

Answer



1,1-dichloro-2,2-di(4-chlorophenyl)ethene

**Answers to end of chapter questions (on p. 445 in *Chemistry*<sup>3</sup>)**

1. Draw skeletal structures of the following compounds:

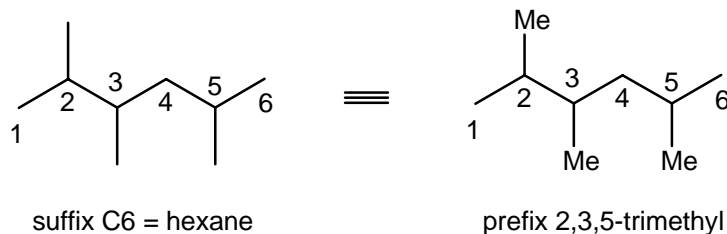
(a) 2,3,5-trimethylhexane

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct!

Solution

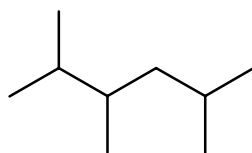
1. This molecule is an alkane. The longest number of continuous carbon atoms is six (**hexane**). Draw out this carbon chain.
2. There are three methyl (Me) groups at carbons-2, -3 and -5.



3. Name the structure that you have drawn (just to double check). This structure is 2,3,5-trimethylhexane.

Answer

This structure is 2,3,5-trimethylhexane.



2,3,5-trimethylhexane

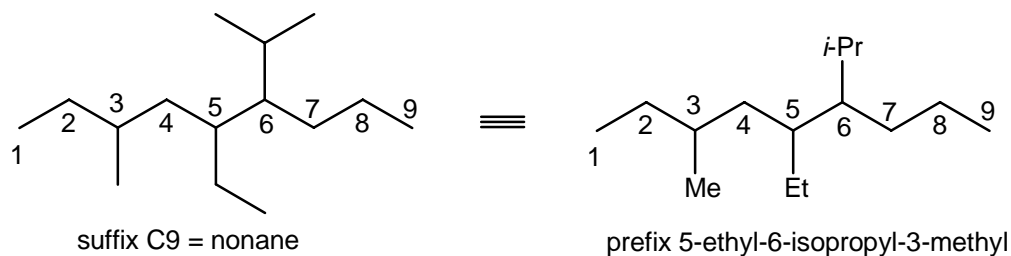
(b) 5-ethyl-6-isopropyl-3-methylnonane.

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct!

Solution

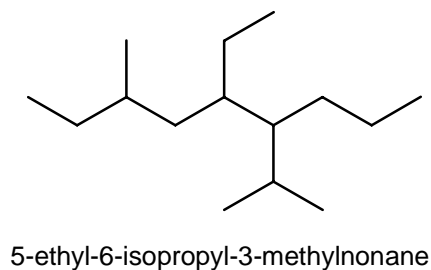
1. This molecule is an alkane. The longest number of continuous carbon atoms is nine (**nonane**). Draw out this carbon chain.
2. There are three substituents, a methyl (Me) group at carbon-3, an ethyl (Et) at carbon-5, and an isopropyl (*i*-Pr) group at carbon-6.



3. Name the structure that you have drawn (just to double check). This structure is 2,3,5-trimethylhexane.

Answer

This structure is 2,3,5-trimethylhexane.



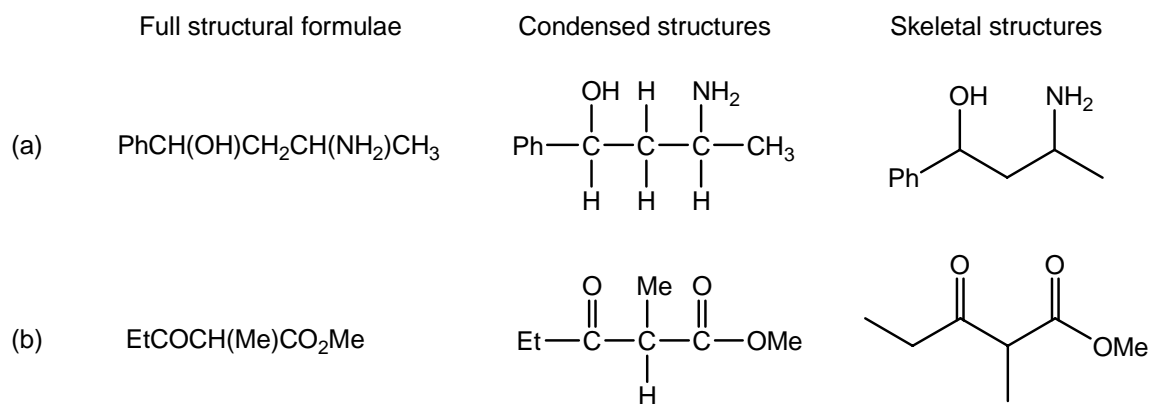
3. Draw skeletal structures of the following compounds:



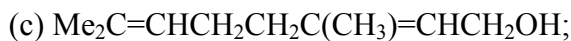
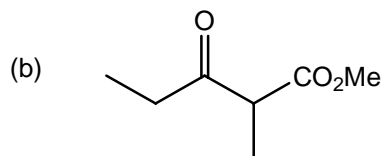
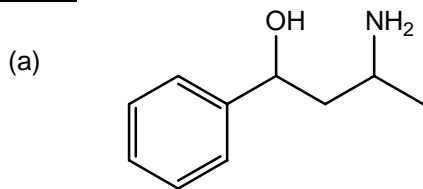
### Strategy

In order to draw out these molecules as skeletal structures, their full structural formula must first be drawn. These can be easily converted into skeletal structures by omitting the hydrogen atoms attached to carbon atoms. Invariably, skeletal structures are drawn in a *zig-zag* arrangement involving the longest carbon chain.

### Solution



### Answers



### Strategy

In order to draw out this molecule as a skeletal structure, the full structural formula must first be drawn. This can be easily converted into a skeletal structure by omitting the

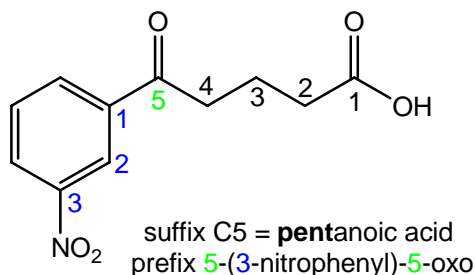


1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct by re-naming it!
4. Re-draw, if necessary, into the required skeletal structure.

### Solution

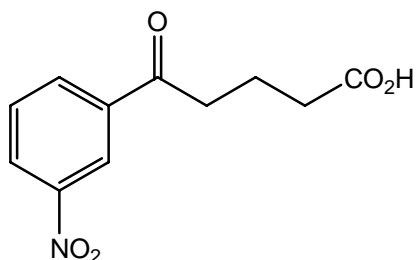
1. The longest number of continuous carbon atoms is five (**pentanoic acid**). Draw out this carbon chain. The suffix of this molecule is -oic (pentano**ic** acid); it is therefore a carboxylic acid. The carboxylic acid group is at carbon-1.
2. There are two different substituents at carbon-5; a 3-nitrophenyl group and an oxo(=O) group (commonly known as a carbonyl group).

5-(3-nitrophenyl)-5-oxopentanoic acid

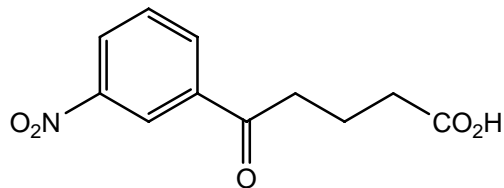


3. This structure is this correct. It is 5-(3-nitrophenyl)-5-oxopentanoic acid.

4. The skeletal structure is:



### Answer



5. Give IUPAC names for the following compounds:

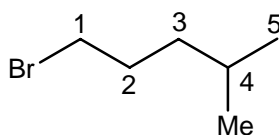
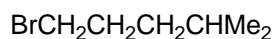


Strategy

1. Identify the longest continuous carbon chain. All alkane names end with -ane.
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has **FIVE** carbon atoms; therefore its suffix is **pentane**.
2. For this molecule, the carbon atoms are numbered from left to right as 1-bromo-4-methyl- has lower numbers than 2-methyl-5-bromo-. [Remember **b**romo comes before **m**ethyl as **b** comes before **m** in the alphabet.]

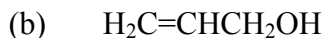


suffix C5 = **pentane**  
 prefix 1-bromo-4-methyl

3. The name of this compound is 1-bromo-4-methylpentane.

Answer

1-Bromo-4-methylpentane

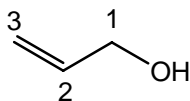


Strategy

1. Identify the longest continuous carbon chain. Draw out this chain. This molecule is an alcohol, so its suffix will be -ol (*c.f.* alcohol).
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has **THREE** carbon atoms; and as this molecule is an alcohol, its suffix is **propanol**.
2. As this molecule is propanol, the -OH group is at position-1. The remaining functional group, alkene, is at carbon-2 ( $\rightarrow$ 3).



suffix C3 = **propanol**  
functional group = 2-ene

3. The name of this compound is prop-2-en-1-ol.

Answer

Prop-2-en-1-ol

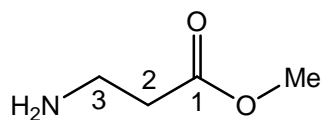
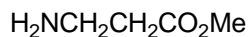


Strategy

1. Identify the longest continuous carbon chain. Draw out this chain. This molecule is an ester, so its suffix will be -oate.
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has **THREE** carbon atoms; and as this molecule is an **ester**, its suffix is **propanoate**.
2. This molecule is a **methyl** ester. The C=O group is at position-1. The remaining functional group, amine, is at carbon-3.

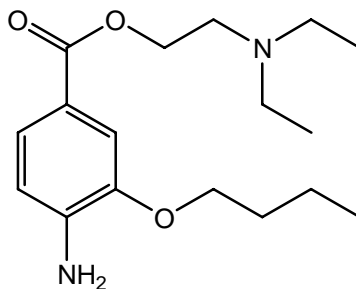


suffix C3 = **propanoate**  
prefix = 3-amino

3. The name of this compound is methyl-3-aminopropanoate.

Answer

Methyl-3-aminopropanoate



ambucaine

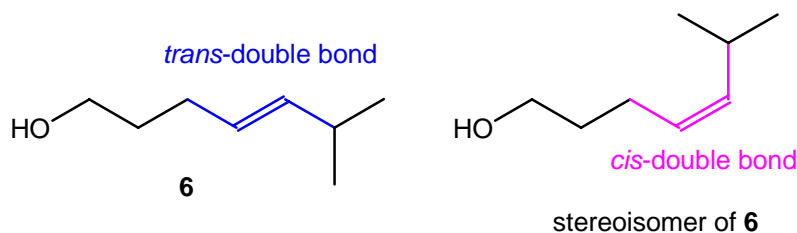
7. The hot spicy flavour of chilli peppers of the *Capsicum* family is due mainly to a compound called capsaicin. The following questions relate to the synthesis of capsaicin shown below.

(a) Draw a skeletal structure of the stereoisomer of alkene **6**.

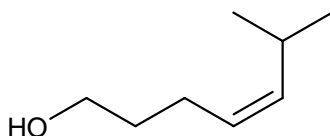
Strategy

Molecule **6** is a di-substituted alkene and has *trans*-stereochemistry. The remaining stereoisomer of **6** must have *cis*-stereochemistry. [A *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.]

Solution



Answer



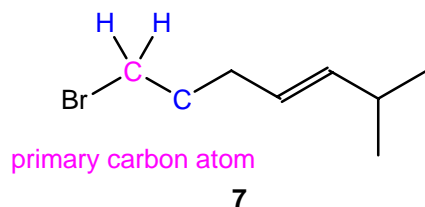
- (b) In compound **7**, is the bromine bonded to a primary, secondary, or tertiary carbon atom?

Strategy

To determine whether this carbon atom bonded to the bromine atom is primary, secondary or tertiary, count the number of carbon atoms attached to it.

Solution

There is one carbon atom attached to the carbon atom bonded to the bromine atom. This carbon atom is primary.

Answer

The bromine atom is attached to a primary carbon atom.

- (c) For the synthesis of compound **8**,  $\text{NaCH}(\text{CO}_2\text{Et})_2$  is prepared from  $\text{CH}_2(\text{CO}_2\text{Et})_2$ , which has the common name diethyl malonate. Draw a skeletal structure of diethyl malonate and give the IUPAC name.

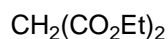
Strategy

In order to draw this molecule as a skeletal structure, the full structural formula must first be drawn out. This can be easily converted into its skeletal structure by omitting the hydrogen atoms attached to carbon atoms. Invariably, skeletal structures are drawn in a *zig-zag* arrangement involving the longest carbon chain.

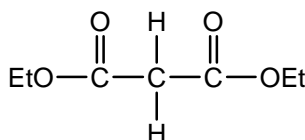
To name this compound: identify the longest continuous carbon chain. Draw out this chain. This molecule contains two esters, so its suffix will be **-ate** and its prefix will be **di-**. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

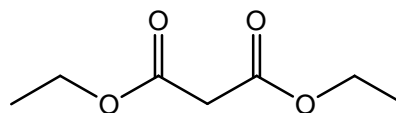
Full structural formula



Condensed structure



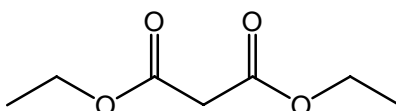
Skeletal structure



The longest continuous carbon chain has **THREE** carbon atoms; and as this molecule is a **diester**, its suffix will be **propanedioate**. This molecule is a **diethyl** ester.

The full IUPAC name of this molecule is diethyl propanedioate. Interesting, it could have also been called diethyl propane-1,3-dioate, but as there is no ambiguity of where these diesters are located, the locant “-1,3-“ is not required.

Answer



diethyl propanedioate

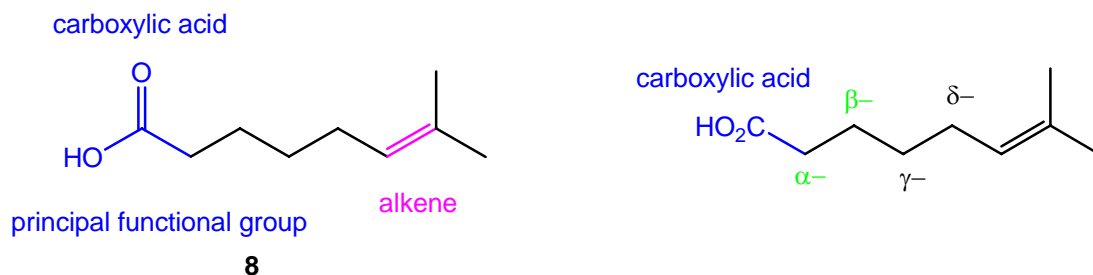
(d) Draw the structure of compound **8**, and indicate the  $\alpha$ - and  $\beta$ -carbon atoms.

Strategy

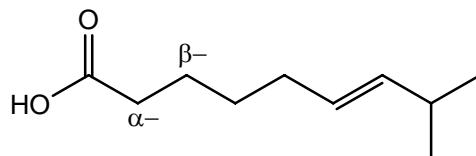
The carbon atoms of a given molecule can be labelled sequentially away from its principle functional group; usually these carbon atoms are labelled using the Greek alphabet [*e.g.*, alpha- ( $\alpha$ -), beta- ( $\beta$ -), gamma ( $\gamma$ -), delta ( $\delta$ -) and so on ...].

Solution

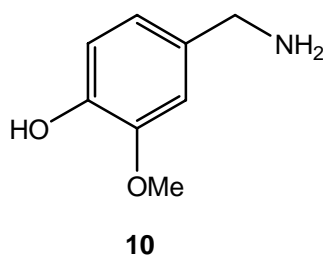
Molecule **8** contains two functional groups; the carboxylic acid is the principal functional group and the alkene is the secondary functional group; the  $\alpha$ -carbon atom is adjacent to the principal functional group, and so on.



Answer



(e) Give the IUPAC name for compound **10**.



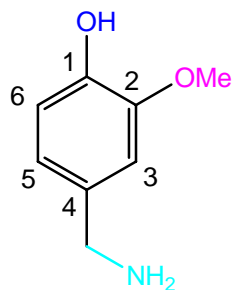
Strategy

1. Draw out this trisubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around the benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned and have the lowest possible numbers.
3. Write out the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The principal functional group is the phenol group (ArOH).
2. The carbon atom bearing this phenolic (OH) group is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of any substituents. There are two substituents; the methoxy (-OMe) and aminomethyl (NH<sub>2</sub>CH<sub>2</sub>-) groups are at carbons-2 and -4, respectively.

principal functional group



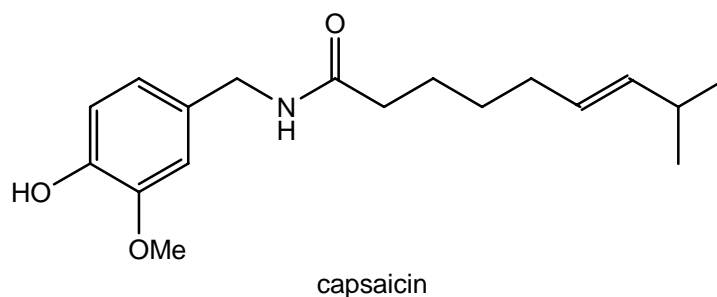
4-(aminomethyl)-2-methoxyphenol

3. This molecule is 4-(aminomethyl)-2-methoxyphenol. [Remember **a**minomethyl comes before **m**ethoxy as **a** comes before **m** in the alphabet.]

Answer

4-(aminomethyl)-2-methoxyphenol

- (f) Name all of the functional groups in capsaicin.

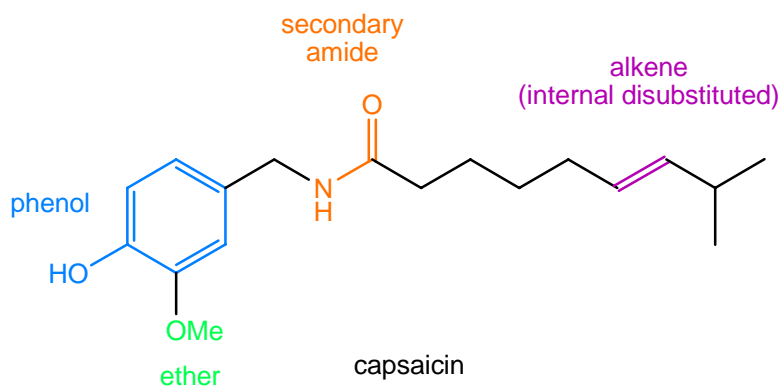


capsaicin

Strategy

This molecule contains four functional groups. There are three obvious functional groups, the ether group (ArOMe), the secondary amide (RCO<sub>2</sub>NHR) and the substituted phenol (ArOH). The remaining functional group is an alkene.

Solution



Answer

Capsaicin contains FOUR functional groups; phenol, ether, secondary amide and alkene.

Solutions provided by J. Eames (j.eames@hull.ac.uk)