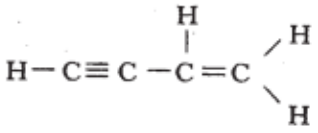
AH Exercise 2.1a

Molecular Orbitals

2003 AH MC32 (81%) and 2006 AH MC28 (79%)

32. Which line in the table has the correct number and type of bonds in



	Number of σ–bonds	Number of π–bonds
A	7	3
B	5	3
C	5	2
D	5	5

2012 AH MC30 (88%)

30. Carbon dioxide has the following structure.

O = C = O

Which line in the table shows the correct numbers of σ and π bonds in a molecule of carbon dioxide?

	Number of σ bonds	**Number of π bonds**
A	0	2
B	2	2
C	4	0
D	0	4

2011 AH MC30 (62%)

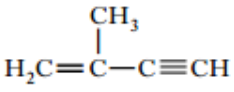
30. Pyridine, C_5H_5N, has the following structure:

Which line in the table shows the correct numbers of σ and π bonds in a molecule of pyridine?

	Number of σ bonds	**Number of π bonds**
A	3	11
B	6	3
C	11	3
D	12	3

2009 AH MC26 (70%)

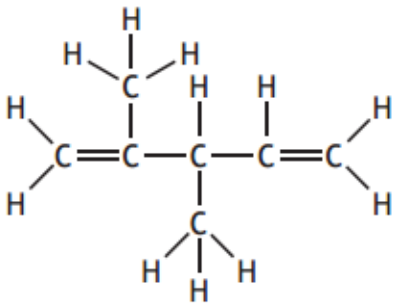
26. Which line in the table is correct for the following hydrocarbon?



	Number of σ bonds	Number of π bonds
A	4	3
B	8	5
C	10	2
D	10	3

2016 AH MC12 (92%)

12. Which line in the table has the correct number and type of bonds in the structure shown?



	Number of σ-bonds	*Number of π-bonds*
A	2	18
B	4	16
C	16	4
D	18	2

2007 AH MC31 (72%) and 2014 AH MC26 (86%) and 2014 revAH MC15 (48%)

31. The end-on overlap of two atomic orbitals lying along the axis of a bond is known as

A hybridisation

B a sigma bond

C a pi bond

D a double bond.

2012 AH MC29 (56%)

29. Hybrid orbitals can be formed by the mixing of s and p orbitals.

Which of the following hybrid orbitals are most likely to be involved in the bonding in ethyne?

A sp

B sp^2

C sp^3

D s^2p

2006 AH MC29 (78%)

29. Which of the following best describes the bonding in alkanes?

A sp^2 hybridisation of the carbon atoms giving sigma bonds only

B sp^2 hybridisation of the carbon atoms giving sigma and pi bonds

C sp^3 hybridisation of the carbon atoms giving sigma bonds only

D sp^3 hybridisation of the carbon atoms giving sigma and pi bonds

2005 AH MC36 (69%) and 2011 AH MC28 (79%)

36. Which of the following best describes the bonding in ethane?

A sp^2 hybridisation of the carbon atoms giving sigma bonds only

B sp^2 hybridisation of the carbon atoms giving sigma and pi bonds

C sp^3 hybridisation of the carbon atoms giving sigma bonds only

D sp^3 hybridisation of the carbon atoms giving sigma and pi bonds

2010 AH MC28 (52%)

28. The sideways overlap of two parallel atomic orbitals lying perpendicular to the axis of the bond is known as

A hybridisation

B a pi bond

C a sigma bond

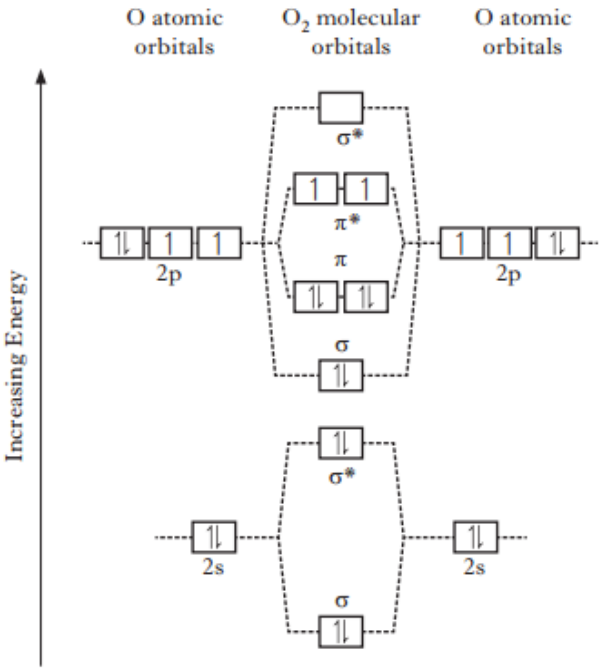
D a double bond.

2015 revAH MC10 (57%)

10. The stability of a covalent bond is related to its bond order, which can be defined as follows:

bond order = $\frac{1}{2}$(number of bonding electrons – number of anti-bonding electrons)

The molecular orbital diagram for oxygen is shown. The anti-bonding orbitals are denoted by *.



The bond order for a molecule of oxygen is

A 0

B 1

C 2

D 3.

2015 revAH MC18 (60%)

18. Lycopene and ß-carotene are coloured organic compounds found in ripened tomatoes. Both absorb light in the visible region. Lycopene is red and ß-carotene is orange.

Which of the following statements is true about the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) in lycopene and ß-carotene?

A ß-Carotene has a higher energy gap between HOMO and LUMO than lycopene.

B Lycopene has a higher energy gap between HOMO and LUMO than ß-carotene.

C ß-Carotene has the same energy gap between HOMO and LUMO as lycopene.

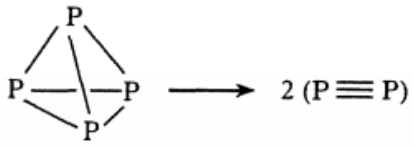
D The colour of ß-carotene and lycopene is not affected by the energy gap between HOMO and LUMO.

2001 AH L9c

9. When phosphorus is heated the following transition occurs at 800 °C.

$$P_4(g) \rightarrow 2P_2(g)$$

Using structural formulae, the transition may be represented as:



(*c*) How many pi (π) bonds are present in a P_2 molecule? **1**

2002 AH L4b

4. Difluoromethanimine, FN = CHF, can exist in two isomeric forms.

When a sample of the *trans*-isomer was dissolved in an organic solvent at 22 °C it was slowly converted into the *cis*-isomer. After 7 days, 95% of the *trans*-isomer had been converted and no further conversion occurred thereafter.

(*b*) Difluoromethanimine contains a pi bond.

Explain how a pi bond is formed. **1**

2008 AH L10b

10. A mixture of butan-1-ol and butan-2-ol can be synthesised from 1-bromobutane in a two stage process.

$$CH_3CH_2CH_2CH_2Br \xrightarrow[\textbf{Stage 1}]{KOH/C_2H_5OH} CH_3CH_2CH{=}CH_2 \xrightarrow[\textbf{Stage 2}]{H_2O/H^+} \begin{matrix}\text{butan-1-ol}\\+\\\text{butan-2-ol}\end{matrix}$$

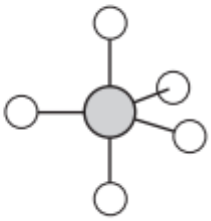
(*b*) The bonding in but-1-ene can be described in terms of sp^2 and sp^3 hybridisation and sigma and pi bonds.

(i) What is meant by sp^2 hybridisation? **1**

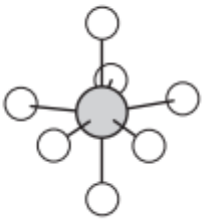
(ii) What is the difference in the way atomic orbitals overlap to form sigma and pi bonds? **1**

2009 AH L12c

12. Many interhalogen compounds exist. Two of these are iodine pentafluoride and iodine heptafluoride.



IF_5



IF_7

(*c*) In iodine heptafluoride, there are seven I–F bonds in which iodine uses sp^3d^3 hybrid orbitals.

Suggest which hybrid orbitals iodine uses in iodine pentafluoride, in which there are five I–F bonds. **1**

2013 revAH L1c

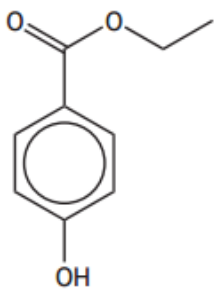
1. The electronic configuration of a carbon atom is $1s^22s^22p^2$.

(*c*) Explain what is thought to take place when carbon atoms form four equivalent single bonds in methane. **2**

2016 AH L9(iii)

9. Parabens are used as preservatives in cosmetics, pharmaceutical products and foods. Parabens are esters of 4-hydroxybenzoic acid.

One common paraben used as a food preservative is ethylparaben.



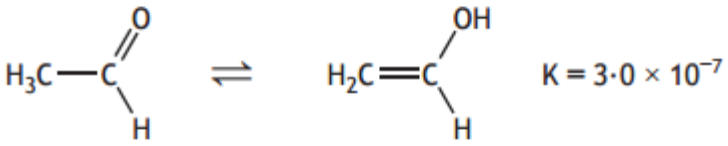
ethylparaben

(a) Ethylparaben is an aromatic compound containing both sigma and pi bonds.

(iii) Describe how pi bonds form. **1**

7. Aldehydes and ketones can exist in two forms, a keto form and an enol form.

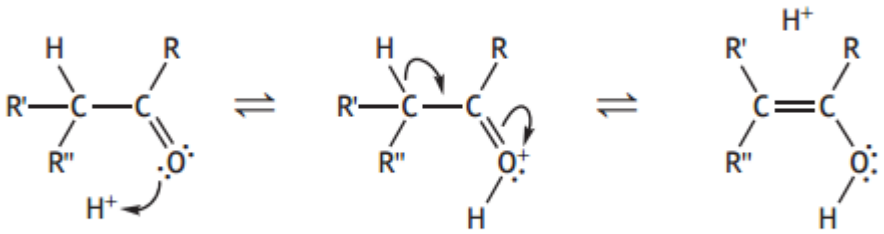
For example, the aldehyde ethanal exists in equilibrium with its enol form, ethenol.



ethanal (keto form) ethenol (enol form)

These two different molecules are known as tautomers.

(c) A possible mechanism for acid-catalysed enolisation is shown below, where R, R' and R" are alkyl groups.



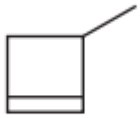
Using structural formulae and curly arrow notation, show a possible mechanism for the acid-catalysed enolisation of 3-methylpentan-2-one. **3**

AH Exercise 2.1b

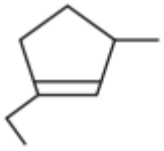
Molecular Structures

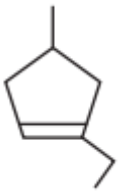
2010 AH MC29 (51%)

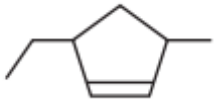
29. If the structure of 3-methylcyclobutene can be represented by

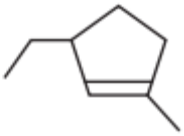


then the structure of 1-ethyl-3-methylcyclopentene will be represented by

A 

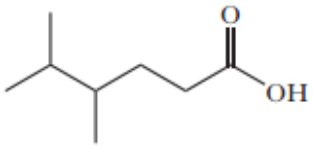
B 

C 

D 

2015 revAH MC11 (82%)

11.



The name of the compound shown above is

A 2,3-dimethylpentanoic acid

B 2,3-dimethylhexanoic acid

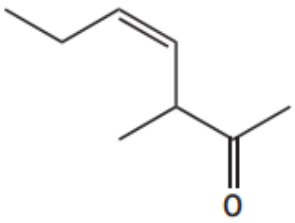
C 4,5-dimethylhexanoic acid

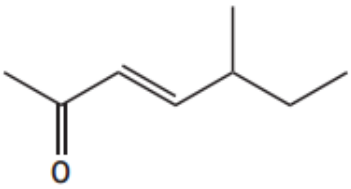
D 4,5,5-trimethylpentanoic acid.

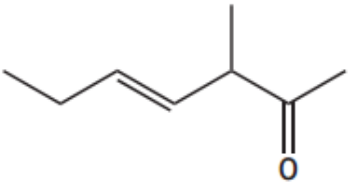
2016 AH MC13 (71%)

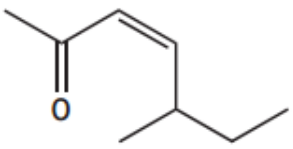
13. 5-Methylhept-3-ene-2-one is an aroma molecule found in some types of tea.

Which of the following shows a structural formula for the *trans*-isomer of 5-methylhept-3-ene-2-one?

A 

C 

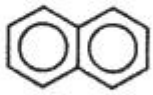
B 

D 

2003 AH MC36 (92%)

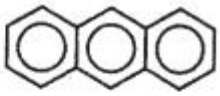
36. Naphthalene and anthracene are examples of polycyclic aromatic hydrocarbons.

Naphthalene:
Structural formula



Molecular formula $C_{10}H_8$

Anthracene:
Structural formula



The molecular formula of anthracene is

A $C_{14}H_{10}$

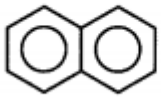
B $C_{12}H_{10}$

C $C_{14}H_{12}$

D $C_{12}H_{12}$.

2006 AH MC35 (20%)

35. Naphthalene, $C_{10}H_8$, has the following structure.



The number of moles of hydrogen gas required for the complete hydrogenation of 12·8 g naphthalene will be

A 0·1

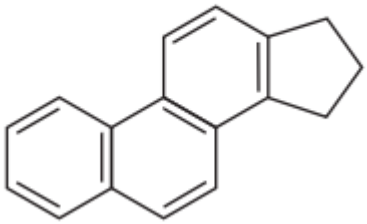
B 0·4

C 0·5

D 0·8.

2009 AH MC25 (56%)

25.



What is the molecular formula for the above structure?

A $C_{17}H_{11}$

B $C_{17}H_{14}$

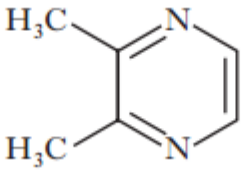
C $C_{17}H_{17}$

D $C_{17}H_{20}$

2013 revAH L7b

7. The dominant flavours of chocolate are due to molecules called substituted pyrazines. These are produced when sugars and amino acids react during the roasting of cocoa beans.

An example is 2,3-dimethylpyrazine

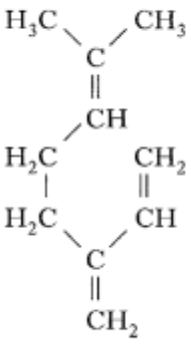


This compound is responsible for the nutty flavour of chocolate. Other substances responsible for the distinctive smell of chocolate are aldehydes including phenylethanal, 2-methylbutanal and 3-methylbutanal.

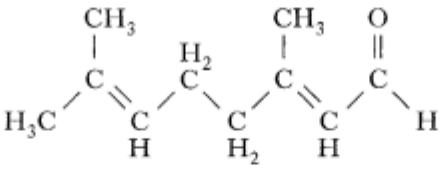
(*b*) Draw a skeletal formula for 2-methylbutanal and circle the asymmetric carbon present. **2**

2002 AH L12d

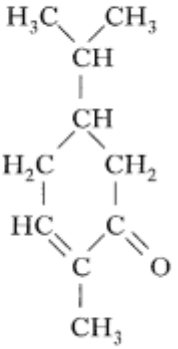
12. Myrcene, citral and carvone belong to a large group of compounds known as terpenes.



myrcene

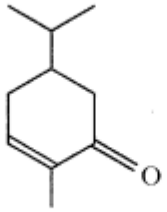


citral



carvone

(*d*) The skeletal structural formula of carvone is



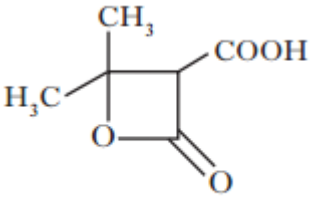
Draw the skeletal structural formula of citral. **1**

2011 AH L11b(i)

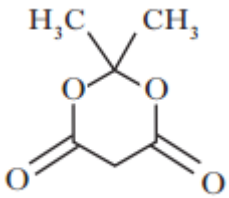
11. Meldrum's acid is a chemical named after the Scotsman, Andrew N. Meldrum who was the first to produce it.

Microanalysis showed that Meldrum's acid has a composition, by mass, of 50% C, 5·6% H, 44·4% O.

b) Meldrum initially thought the structure to be that shown as Compound A shown below. However, it was shown later that the actual structure was an isomer of A and is shown below as compound B.



Compound A



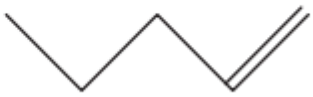
Compound B

(i) What is the molecular formula of **A** and **B**? **1**

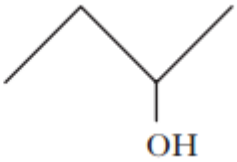
2012 AH L12a

12. Skeletal structural formulae are used to show structures of molecules more simply than full structural formulae.

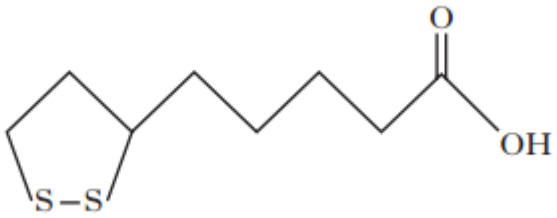
For example, pent-1-ene can be represented as



and butan-2-ol as



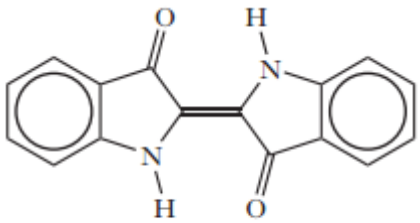
Lipoic acid has recently been used as a food supplement. The skeletal structural formula of lipoic acid is shown below.



(*a*) Write the molecular formula of lipoic acid. **1**

2015 AH L9a+9c and 2015 revAH L9a+9b+9d(ii)

9. The blue colour of denim jeans comes from a dye known as indigo.



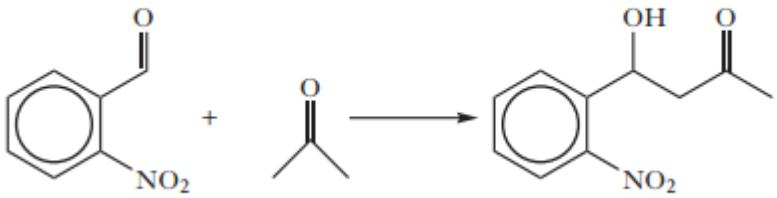
indigo

The synthesis of this dye involves a series of complex chemical reactions.

(*a*) What structural feature of indigo dye allows it to absorb light within the visible region of the electromagnetic spectrum? **1**

(*b*) Why does a dye, such as indigo, appear blue when viewed in daylight? **1**

(*d*) The first step in the synthesis of indigo is the reaction of 2-nitrobenzaldehyde with propanone.



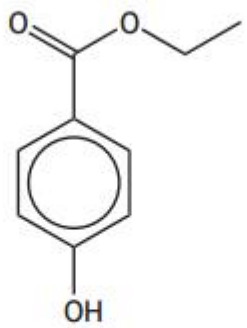
2-nitrobenzaldehyde propanone 4-hydroxy-4-(2-nitrophenyl)butan-2-one

(ii) Suggest the type of chemical reaction taking place during this step of the synthesis. **1**

2016 AH L9a(i)

9. Parabens are used as preservatives in cosmetics, pharmaceutical products and foods. Parabens are esters of 4-hydroxybenzoic acid.

One common paraben used as a food preservative is ethylparaben.



ethylparaben

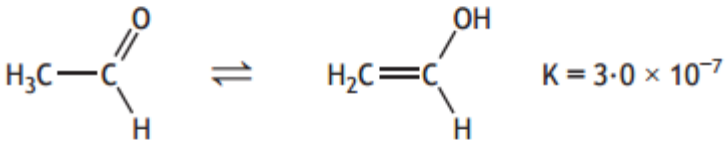
(a) Ethylparaben is an aromatic compound containing both sigma and pi bonds.

(i) Write the molecular formula for ethylparaben. **1**

2016 AH L7b(iii)

7. Aldehydes and ketones can exist in two forms, a keto form and an enol form.

For example, the aldehyde ethanal exists in equilibrium with its enol form, ethenol.



ethanal (keto form) ethenol (enol form)

These two different molecules are known as tautomers.

(b) 3-Methylpentan-2-one is optically active and exists in equilibrium with its enol tautomer.

(iii) Draw the skeletal formula for 3-methylpentan-2-one. **1**