Molecular Orbitals Past Papers

1. 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.

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

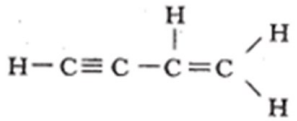
A hybridisation

B a pi bond

C a sigma bond

D a double bond.

3. 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

4. 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?

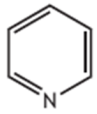
A sp

B sp^2

C sp^3

D s^2p

5. Pyridine has the following structure.



The number of σ bonds in a molecule of pyridine is

A 3

B 6

C 11

D 12

6. 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

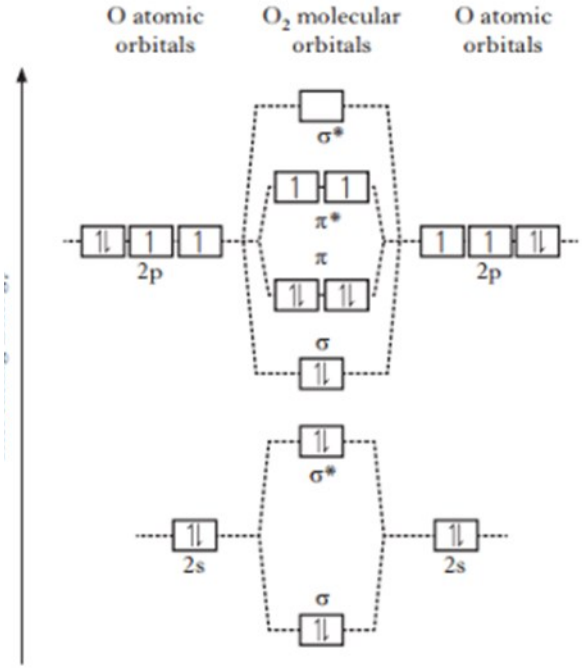
C sp^3 hybridisation of the carbon atoms giving sigma bonds only

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

7. 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

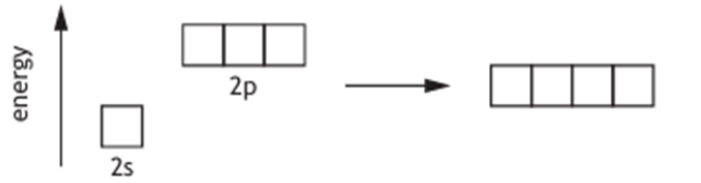
B 1

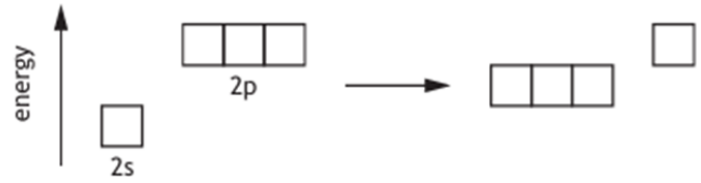
C 2

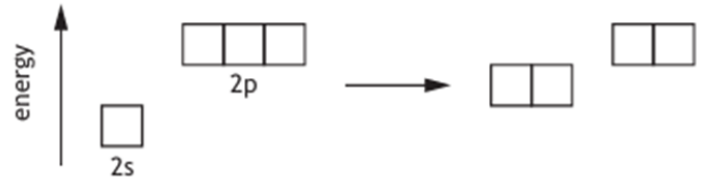
D 3.

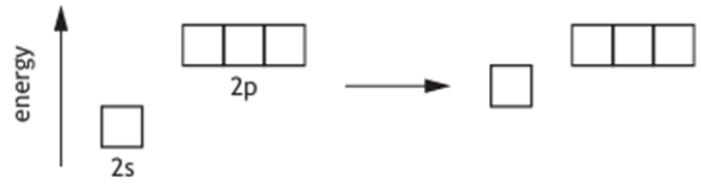
Molecular Orbitals Past Papers

8. Which of the following diagrams represents the hybridisation of orbitals in a carbon atom of ethyne?

A


B


C


D


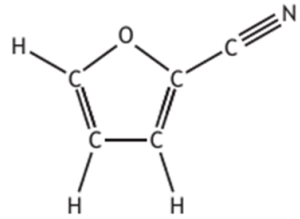
9. Which of the following has the fewest sigma bonds?

A Hexane
B Hex-1-ene
C Hex-1-yne
D Cyclohexane

10. Which of the following molecules contains only sigma bonds?

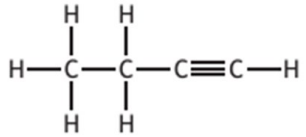
A C_2H_4
B H_2O
C O_2
D N_2

11. The structure of 2-furonitrile is shown.



The number of pi bonds in 2-furonitrile is

A 2
B 3
C 4
D 7.

12.


Which of the following types of hybridisation occur in the above compound?

A sp^3 only
B sp^3 and sp
C sp^3 and sp^2
D sp^3, sp^2 and sp

Molecular Orbitals Past Papers

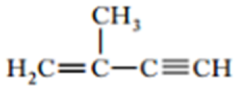
13. Which of the following describes the bonding in ethane?

A sp^2 hybridisation with sigma bonds only.
B sp^3 hybridisation with sigma bonds only.
C sp^2 hybridisation with sigma and pi bonds.
D sp^3 hybridisation with sigma and pi bonds.

14. Which line in the table is correct for a carbon-carbon single bond in an alkane?

	Overlap of atomic orbitals	Symmetry of molecular orbital
A	end-on	symmetrical
B	end-on	asymmetrical
C	side-on	symmetrical
D	side-on	asymmetrical

15. 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

16. 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

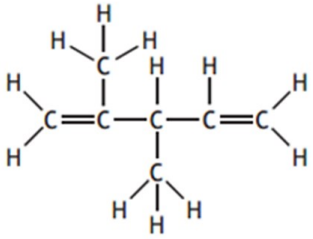
17. Carbon dioxide has the following structure.

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

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



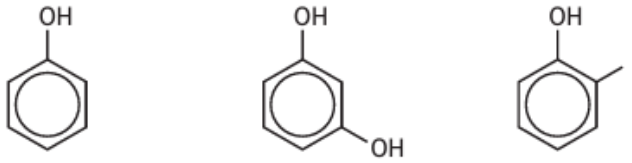
	Number of σ-bonds	*Number of π-bonds*
A	2	18
B	4	16
C	16	4
D	18	2

1

Molecular Orbitals Past Papers

1. Phenols are alcohols with at least one hydroxyl group bonded to a benzene ring.

The structures of some phenols are shown.

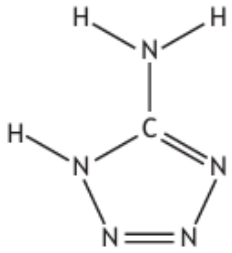


phenol 3-hydroxyphenol 2-methylphenol

The carbon atoms in the benzene ring are sp^2 hybridised giving rise to a π molecular orbital.

State how the π molecular orbital is formed.

2. In some distress flares, 5-aminotetrazole replaces perchlorate ions.



5-aminotetrazole

Determine the number of sigma bonds in a 5-aminotetrazole molecule. **1**

3. Bilirubin is coloured due to the presence of bonding molecular orbitals and antibonding molecular orbitals.

State one difference between a bonding molecular orbital and an antibonding molecular orbital. **1**

4 Bilirubin can have cis or trans isomerism.

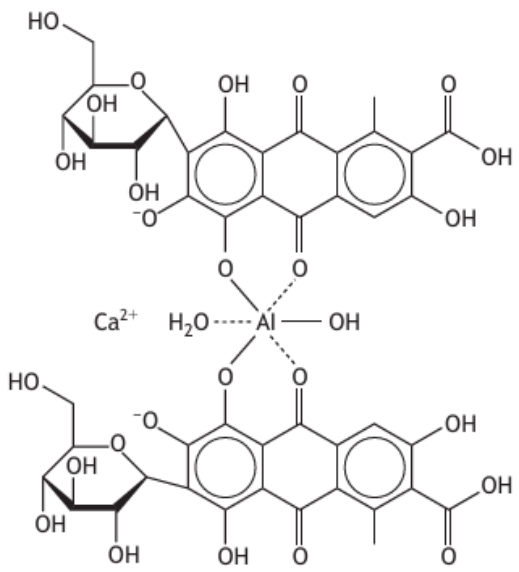
Explain fully why cis and trans isomerism can exist in some compounds with carbon–carbon double bonds. **2**

5 Cyclohexene can be synthesised by an addition reaction between buta-1,3-diene and ethene.

State the type of hybridisation that is adopted by the carbon atoms in buta-1,3-diene. **1**

Molecular Orbitals Past Papers

6 Carmine is a red pigment formed in a precipitation reaction.



carmine

7 The structure shown above contains both pi and sigma bonds.

(i) Explain how a sigma bond is formed.

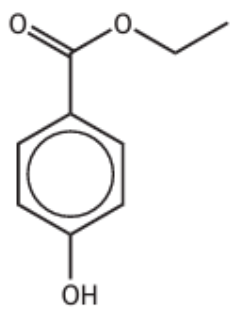
(ii) A pi bond is formed as a result of sp^2 hybridisation.

Explain what is meant by sp^2 hybridisation.

1

8 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

(i) State the type of hybridisation which is adopted by the carbon atoms in the aromatic ring. **1**

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

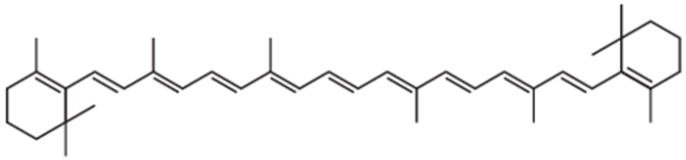
9 Benzene is a colourless, aromatic compound containing a conjugated system of pi (π) bonds.

benzene

State the type of hybridised orbitals found in benzene. **1**

Conjugation systems Past Papers

1. The concentration of an orange solution of carotene was determined by colorimetry.



An appropriate filter was selected and a blank determination carried out using the solvent only.

Which line in the table shows an appropriate filter and solvent for this colorimetric determination?

	Colour of filter	Solvent for blank determination
A	green-blue	water
B	green-blue	hexane
C	orange	water
D	orange	hexane

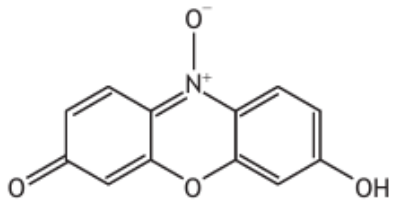
2. Which line in the table is correct for a chromophore that absorbs blue-green light?

	Movement of electrons	Colour observed
A	HOMO to LUMO	blue-green
B	LUMO to HOMO	blue-green
C	HOMO to LUMO	red
D	LUMO to HOMO	red

Conjugation systems Past Papers

1. 3-hydroxyphenol can be used to synthesise the indicator resazurin.

When used as a pH indicator, resazurin changes colour from violet to orange.



resazurin

Explain fully, in terms of the conjugation in the molecule, why resazurin changes colour from violet to orange. **2**

2 Cyclohexene can be synthesised by an addition reaction between buta-1,3-diene and ethene.

Buta-1,3-diene has a conjugated system.

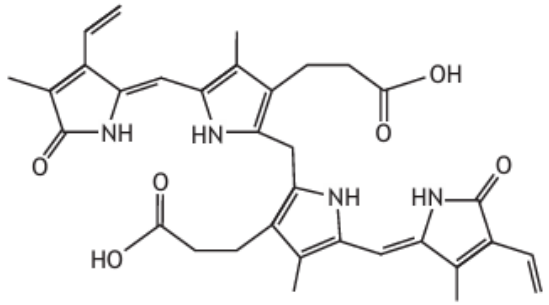
State what is meant by the term conjugated system. **1**

3. Jaundice is a condition caused by a yellow compound in the body called bilirubin.

The structure of bilirubin has two chromophores.

(i) Circle one of the chromophores in the structure of bilirubin below. **1**

(An additional diagram, if required, can be found on *page 34*.)



One treatment for jaundice in new-born babies is to expose them to blue light. This causes the yellow bilirubin to change into compounds that can be excreted by the body.

(ii) Suggest why blue light is used in this treatment. **1**

Conjugation systems Past Papers

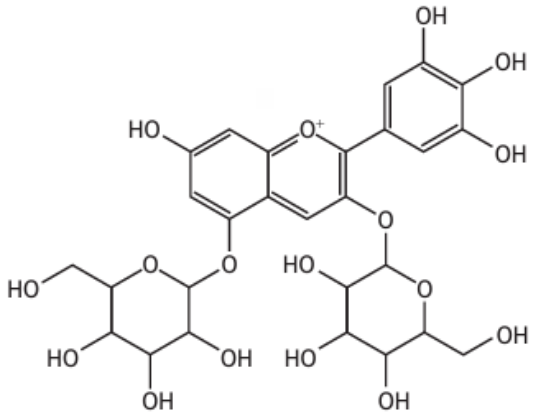
4. The colours of crocus flowers are due to pigments.

(a) The purple colour of crocus petals is due to pigments known as delphinidins.

(i) Delphinidins contain a chromophore.

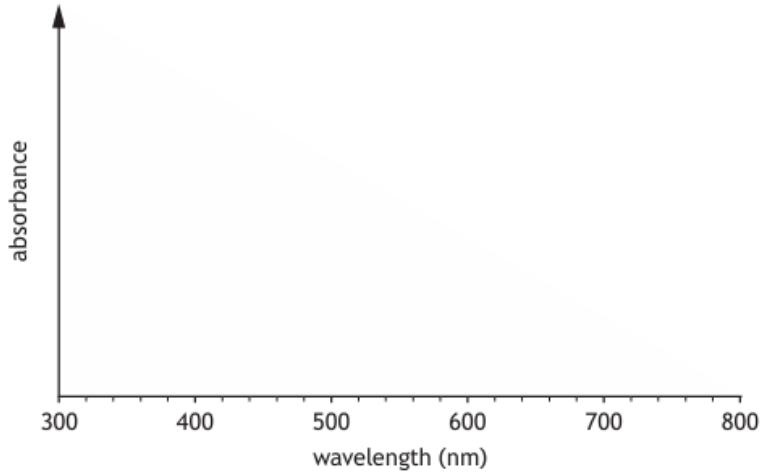
Circle the part of the structure below that contains the chromophore.

(An additional diagram, if required, can be found on *page 34*.)

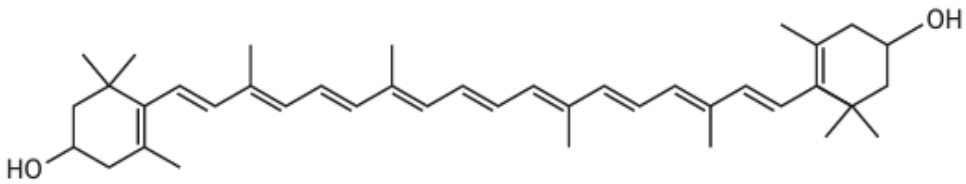


(ii) Complete the diagram below to show an absorption spectrum for a purple delphinidin. **1**

(An additional diagram, if required, can be found on *page 35*.)



(b) Saffron is a spice obtained from crocus flowers. The yellow colour of saffron is partly due to the pigment zeaxanthin.



zeaxanthin

In this structure of zeaxanthin the carbon-carbon double bonds are represented by two lines.

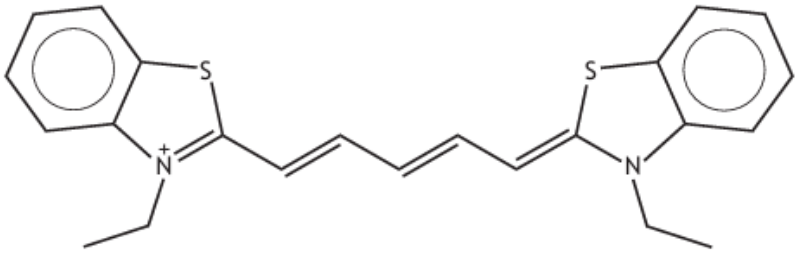
Describe, in terms of overlapping orbitals, what each of the two lines in a double bond represent. **2**

(c) Explain fully why different pigments absorb different wavelengths of light. **2**

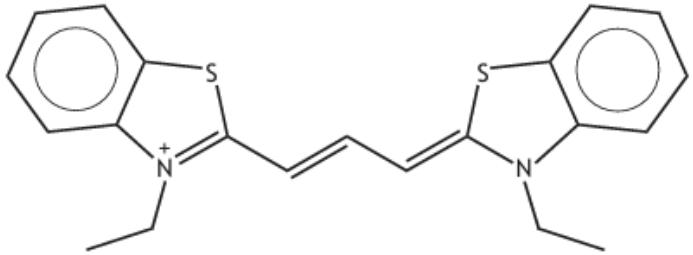
Conjugation systems Past Papers

5. Some dyes contain molecules that are coloured.

The structures of two different dye molecules are shown below.



blue-green

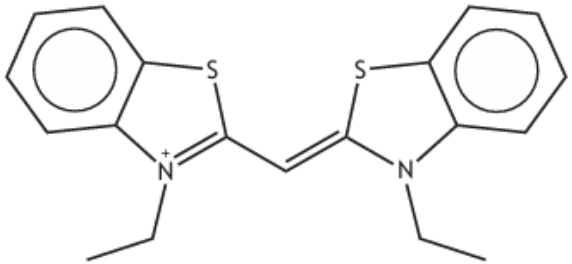


purple

(a) State the structural feature present that is responsible for the colour of these dye molecules. **1**

(b) Explain fully how colour arises in these dye molecules. **2**

(c) A third dye molecule has the following structure.



Explain fully why this dye molecule will absorb a shorter wavelength of light than the other two dye molecules. **2**

Conjugation systems Past Papers

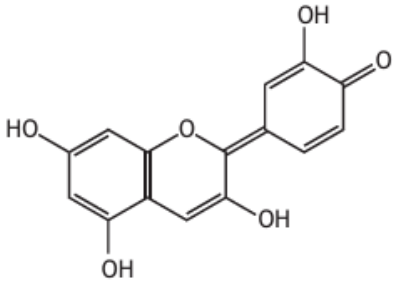
6. Benzene is a colourless, aromatic compound containing a conjugated system of pi (π) bonds.

benzene

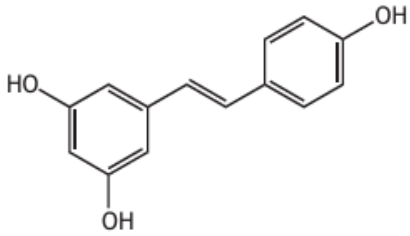
Colour arises in some aromatic compounds due to absorption of visible light.

Explain why the conjugated system in benzene results in absorption of ultraviolet light and not visible light. **2**

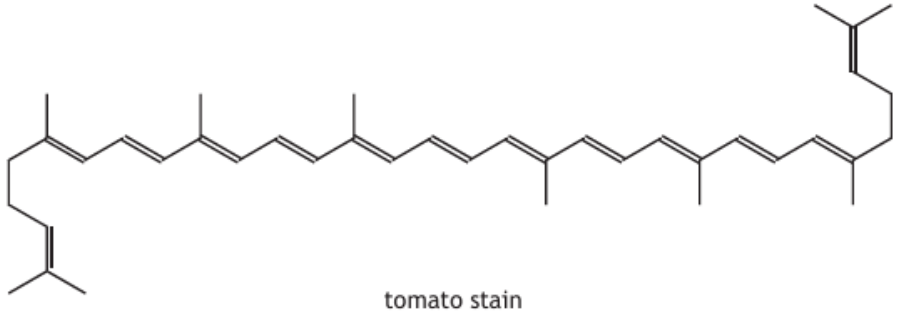
7. Some of the molecules thought to be responsible for the colour of stains are shown.



blackcurrant stain



red wine stain

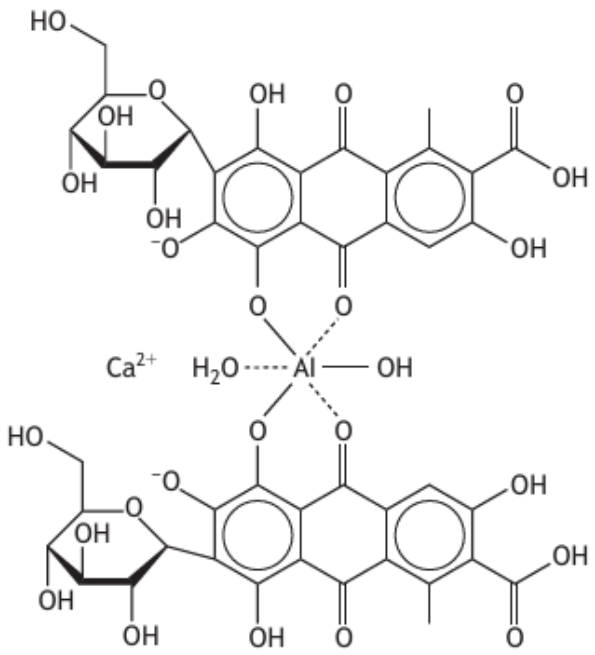


tomato stain

Using your knowledge of chemistry, suggest how the chemicals in a stain remover might work on these stains. **3**

Conjugation systems Past Papers

8. Carmine is a red pigment formed in a precipitation reaction.



carmine

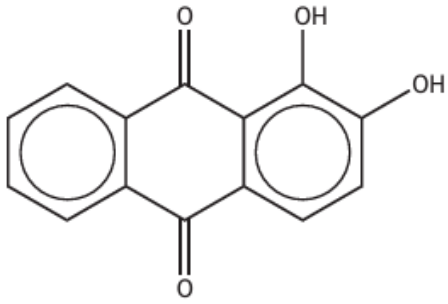
Carmine contains a conjugated system.

Explain fully how this conjugated system gives rise to the red colour of carmine. **2**

9. The use of carmine as a dye was largely abandoned in the nineteenth century.

One of the pigments used to replace carmine is alizarin.

Alizarin can be extracted from the root of a plant using methanol.



alizarin

Explain why methanol is a suitable solvent for this extraction. **1**

Molecular Orbitals Past Papers

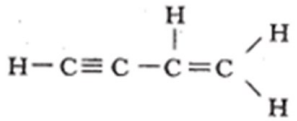
1. The end-on overlap of two atomic orbitals lying along the axis of a bond is known as

A hybridisation
B a sigma bond
C a pi bond
D a double bond.

2. 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.

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



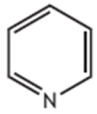
	Number of σ–bonds	Number of π–bonds
A	7	3
B	5	3
C	5	2
D	5	5

4. 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

5. Pyridine has the following structure.



The number of σ bonds in a molecule of pyridine is

A 3
B 6
C 11
D 12

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

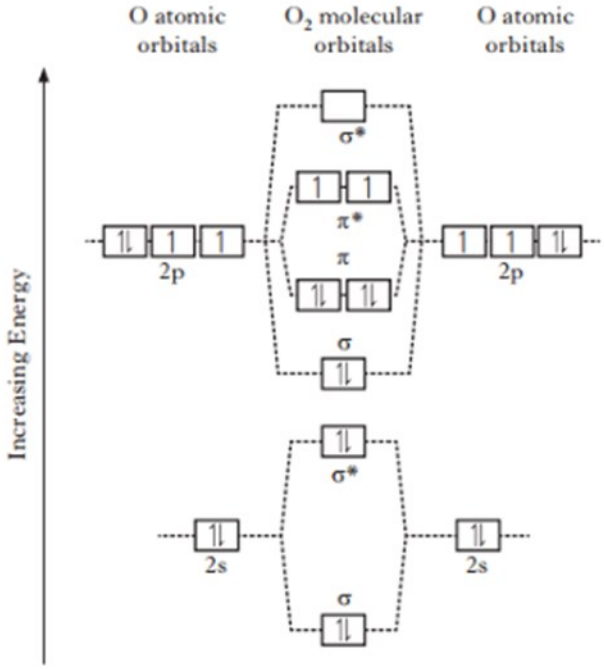
A sp^2 hybridisation of the carbon atoms giving sigma bonds only
B sp^2 hybridisation of the carbon atoms giving sigma and pi bonds
C sp^3 hybridisation of the carbon atoms giving sigma bonds only
D sp^3 hybridisation of the carbon atoms giving sigma and pi bonds

7

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 *.



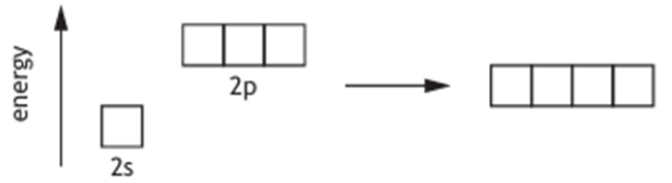
The bond order for a molecule of oxygen is

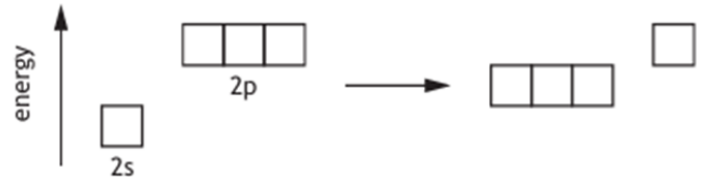
A 0
B 1
C 2
D 3.

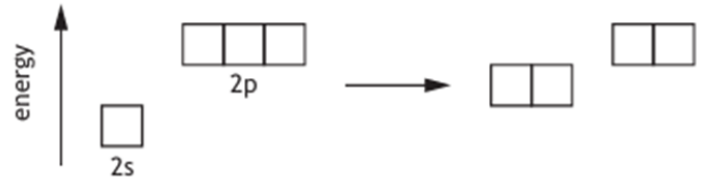
bond order $= \frac{1}{2}(10-6) = \frac{1}{2}(4) = 2$

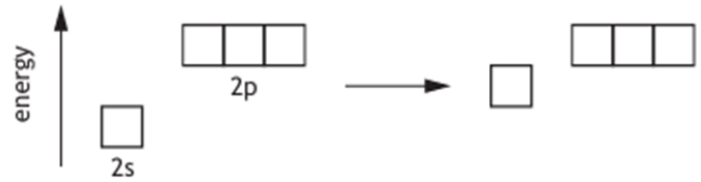
Molecular Orbitals Past Papers

8. Which of the following diagrams represents the hybridisation of orbitals in a carbon atom of ethyne?

A


B


C


D


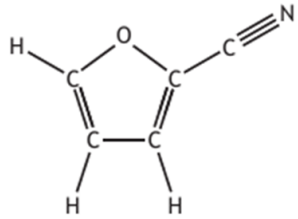
9. Which of the following has the fewest sigma bonds?

A Hexane
B Hex-1-ene
C Hex-1-yne
D Cyclohexane

10. Which of the following molecules contains only sigma bonds?

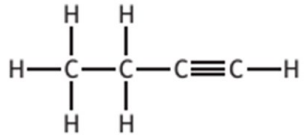
A C_2H_4
B H_2O
C O_2
D N_2

11. The structure of 2-furonitrile is shown.



The number of pi bonds in 2-furonitrile is

A 2
B 3
C 4
D 7.

12.


Which of the following types of hybridisation occur in the above compound?

A sp^3 only
B sp^3 and sp
C sp^3 and sp^2
D sp^3, sp^2 and sp

Molecular Orbitals Past Papers

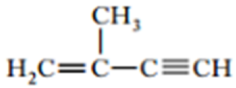
13. Which of the following describes the bonding in ethane?

A sp^2 hybridisation with sigma bonds only.
B sp^3 hybridisation with sigma bonds only.
C sp^2 hybridisation with sigma and pi bonds.
D sp^3 hybridisation with sigma and pi bonds.

14. Which line in the table is correct for a carbon-carbon single bond in an alkane?

	Overlap of atomic orbitals	Symmetry of molecular orbital
A	end-on	symmetrical
B	end-on	asymmetrical
C	side-on	symmetrical
D	side-on	asymmetrical

15. 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

16. 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

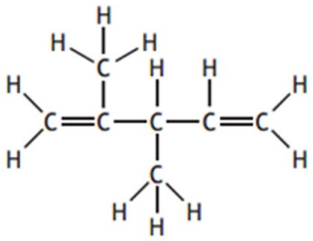
17. Carbon dioxide has the following structure.

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

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



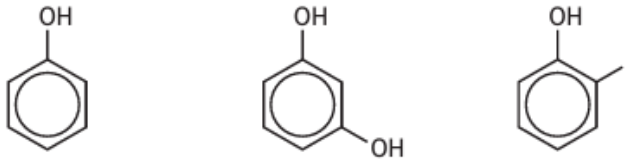
	Number of σ-bonds	*Number of π-bonds*
A	2	18
B	4	16
C	16	4
D	18	2

1

Molecular Orbitals Past Papers

1. Phenols are alcohols with at least one hydroxyl group bonded to a benzene ring.

The structures of some phenols are shown.



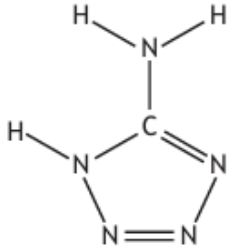
phenol 3-hydroxyphenol 2-methylphenol

The carbon atoms in the benzene ring are sp^2 hybridised giving rise to a π molecular orbital.

State how the π molecular orbital is formed.

Side on overlap of orbitals.

2. In some distress flares, 5-aminotetrazole replaces perchlorate ions.



5-aminotetrazole

Determine the number of sigma bonds in a 5-aminotetrazole molecule. **1**

12

3. Bilirubin is coloured due to the presence of bonding molecular orbitals and antibonding molecular orbitals.

State one difference between a bonding molecular orbital and an antibonding molecular orbital. **1**

Anti-bonding higher energy

OR

Anti-bonding unfilled and bonding filled

4 Bilirubin can have cis or trans isomerism.

Explain fully why cis and trans isomerism can exist in some compounds with carbon–carbon double bonds. **2**

Lack of rotation in carbon to carbon double bonds. (1)

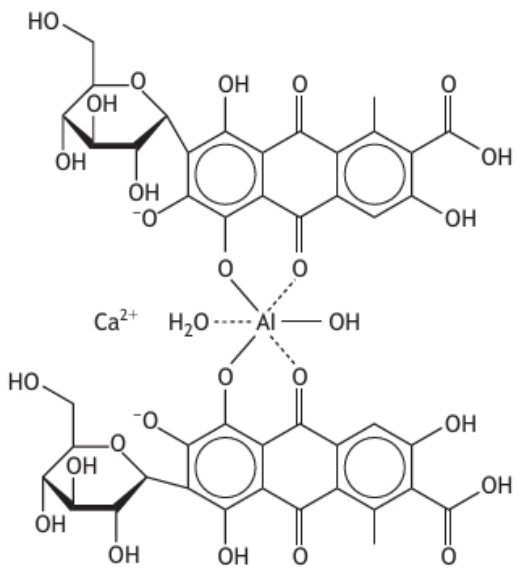
Isomers created when 2 different groups are attached to each carbon atom. (1)

5 Cyclohexene can be synthesised by an addition reaction between buta-1,3-diene and ethene.

State the type of hybridisation that is adopted by the carbon atoms in buta-1,3-diene. **1**

Molecular Orbitals Past papers

6 Carmine is a red pigment formed in a precipitation reaction.



carmine

7 The structure shown above contains both pi and sigma bonds.

(i) Explain how a sigma bond is formed.

End on overlap of orbitals

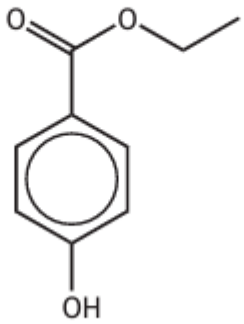
(ii) A pi bond is formed as a result of sp^2 hybridisation.

Explain what is meant by sp^2 hybridisation.

Mixing an s orbital with two p orbitals

8 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

(i) State the type of hybridisation which is adopted by the carbon atoms in the aromatic ring. **1**

sp^2

1

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

9 Benzene is a colourless, aromatic compound containing a conjugated system of pi (π) bonds.

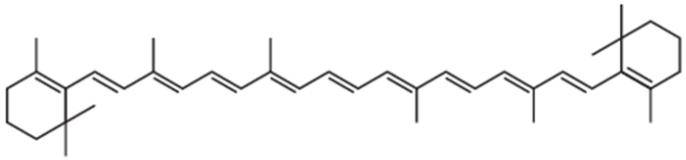
benzene

State the type of hybridised orbitals found in benzene. **1**

sp^2

Conjugation systems Past Papers

1. The concentration of an orange solution of carotene was determined by colorimetry.



An appropriate filter was selected and a blank determination carried out using the solvent only.

Which line in the table shows an appropriate filter and solvent for this colorimetric determination?

	Colour of filter	Solvent for blank determination
A	green-blue	water
B	green-blue	hexane
C	orange	water
D	orange	hexane

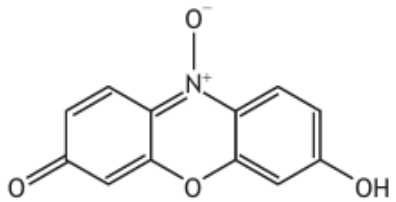
2. Which line in the table is correct for a chromophore that absorbs blue-green light?

	Movement of electrons	Colour observed
A	HOMO to LUMO	blue-green
B	LUMO to HOMO	blue-green
C	HOMO to LUMO	red
D	LUMO to HOMO	red

Conjugation systems Past Papers

1. 3-hydroxyphenol can be used to synthesise the indicator resazurin.

When used as a pH indicator, resazurin changes colour from violet to orange.



resazurin

Explain fully, in terms of the conjugation in the molecule, why resazurin changes colour from violet to orange. **2**

Smaller conjugation system (1)

Larger energy gap between HOMO and LUMO (1)

OR

Absorbs higher energy/ frequency or lower wavelength (1)

2 Cyclohexene can be synthesised by an addition reaction between buta-1,3-diene and ethene.

Buta-1,3-diene has a conjugated system.

State what is meant by the term conjugated system. **1**

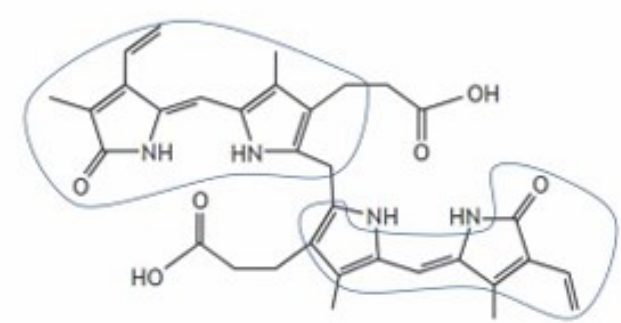
Alternating single and double bonds

3. Jaundice is a condition caused by a yellow compound in the body called bilirubin.

The structure of bilirubin has two chromophores.

(i) Circle one of the chromophores in the structure of bilirubin below. **1**

(An additional diagram, if required, can be found on *page 34*.)



One treatment for jaundice in new-born babies is to expose them to blue light. This causes the yellow bilirubin to change into compounds that can be excreted by the body.

(ii) Suggest why blue light is used in this treatment. **1**

Complementary colour to yellow bilirubin

OR

Bilirubin absorbs blue light

Conjugation systems Past Papers

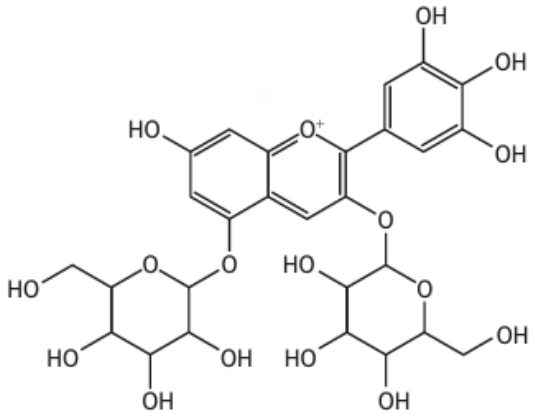
4. The colours of crocus flowers are due to pigments.

(a) The purple colour of crocus petals is due to pigments known as delphinidins.

(i) Delphinidins contain a chromophore.

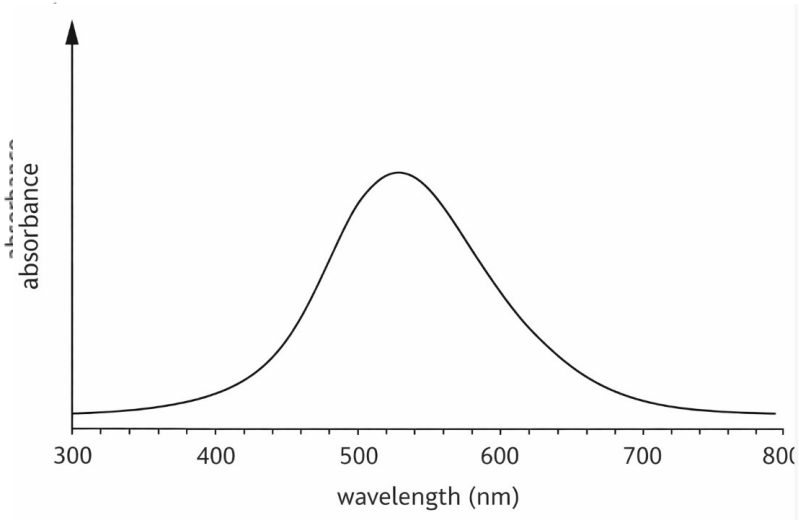
Circle the part of the structure below that contains the chromophore.

(An additional diagram, if required, can be found on *page 34*.)

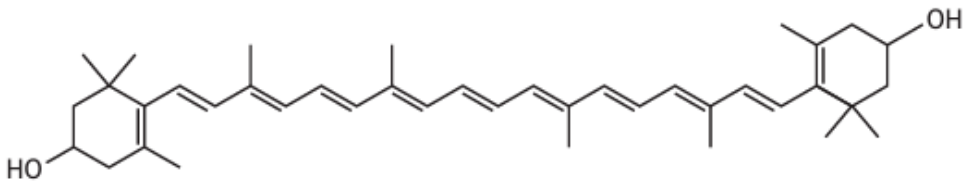


(ii) Complete the diagram below to show an absorption spectrum for a purple delphinidin. 1

(An additional diagram, if required, can be found on *page 35*.)



(b) Saffron is a spice obtained from crocus flowers. The yellow colour of saffron is partly due to the pigment zeaxanthin.



zeaxanthin

In this structure of zeaxanthin the carbon-carbon double bonds are represented by two lines.

Describe, in terms of overlapping orbitals, what each of the two lines in a double bond represent. 2

One line represents end on overlap of sigma bond.

One line represents side on overlap of pi bond

(c) Explain fully why different pigments absorb different wavelengths of light. 2

Smaller conjugation system (1)

Larger energy gap between HOMO and LUMO (1)

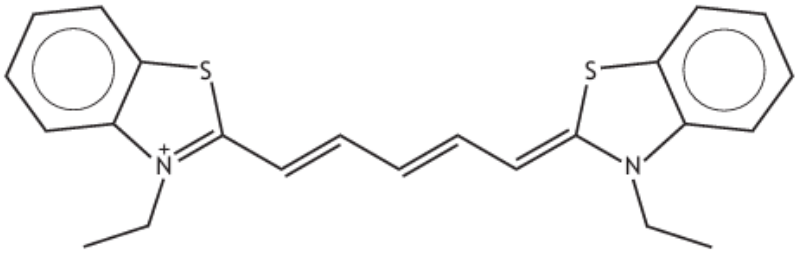
OR

Absorb higher energy/frequency OR lower wavelength

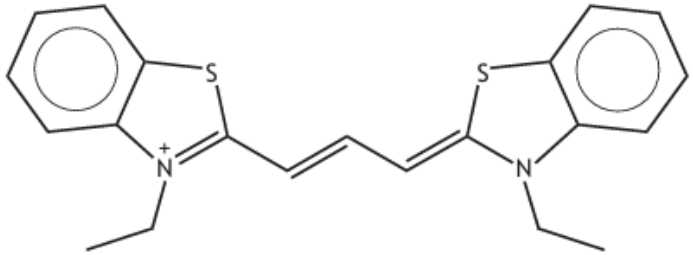
Conjugation systems Past Papers

5. Some dyes contain molecules that are coloured.

The structures of two different dye molecules are shown below.



blue-green



purple

(a) State the structural feature present that is responsible for the colour of these dye molecules. **1**

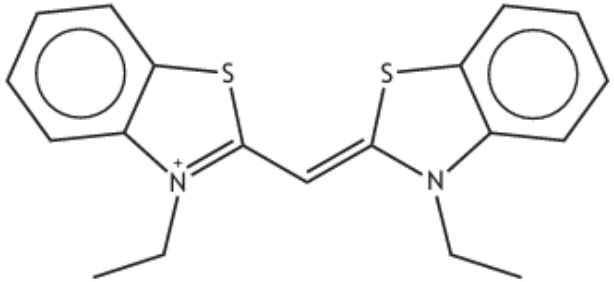
Conjugated system OR alternating double and single bonds.

(b) Explain fully how colour arises in these dye molecules. **2**

Electrons move from HOMO to LUMO. (1)

Absorption of light to promote electron means that light of the complementary colour is seen.

(c) A third dye molecule has the following structure.



Explain fully why this dye molecule will absorb a shorter wavelength of light than the other two dye molecules. **2**

Smaller conjugation system (1)

Larger energy gap between HOMO and LUMO (1)

OR

Absorb higher energy/frequency OR lower wavelength

Conjugation systems Past Papers

6. Benzene is a colourless, aromatic compound containing a conjugated system of pi (π) bonds.

benzene

Colour arises in some aromatic compounds due to absorption of visible light.

Explain why the conjugated system in benzene results in absorption of ultraviolet light and not visible light. **2**

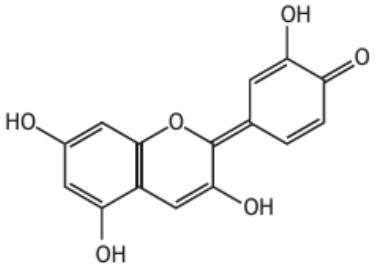
Smaller conjugation system (1)

Larger energy gap between HOMO and LUMO (1)

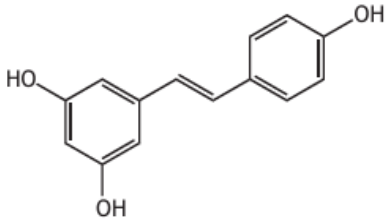
OR

Absorb higher energy/frequency OR lower wavelength

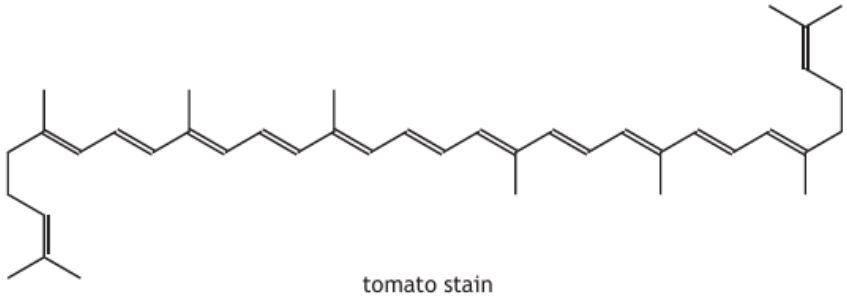
7. Some of the molecules thought to be responsible for the colour of stains are shown.



blackcurrant stain



red wine stain



tomato stain

Using your knowledge of chemistry, suggest how the chemicals in a stain remover might work on these stains. **3**

Stains have larger conjugation system (alternating single & double bonds)

Lower energy gap between HOMO and LUMO

Absorb lower energy/frequency red light

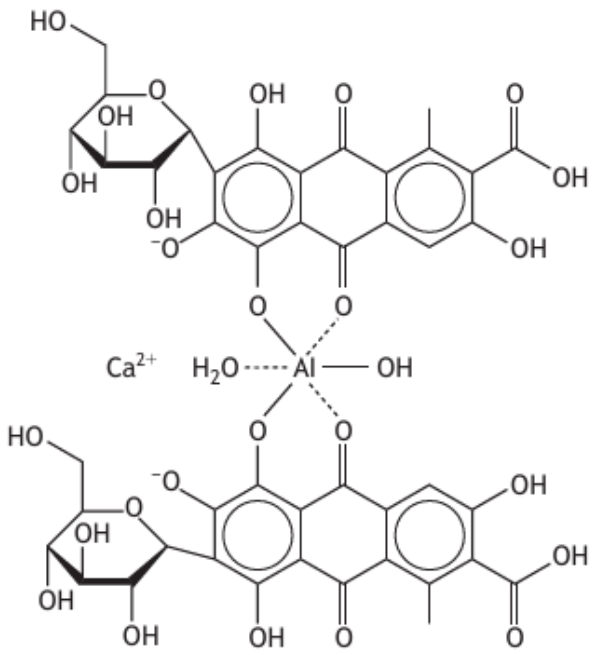
Stain remover breaks compounds into smaller conjugation systems

Higher energy gap between HOMO & LUMO

Absorb higher energy UV light and appears colourless

Conjugation systems Past Papers

8. Carmine is a red pigment formed in a precipitation reaction.



carmine

Carmine contains a conjugated system.

Explain fully how this conjugated system gives rise to the red colour of carmine. **2**

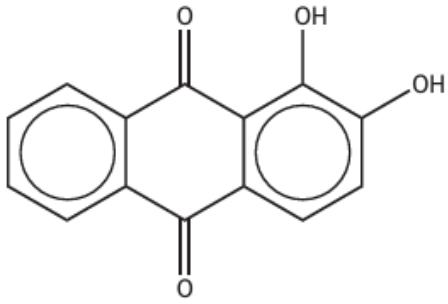
Electrons move from HOMO to LUMO (1)

Blue/green light is absorbed OR complementary colour to red carmine is absorbed

9. The use of carmine as a dye was largely abandoned in the nineteenth century.

One of the pigments used to replace carmine is alizarin.

Alizarin can be extracted from the root of a plant using methanol.



alizarin

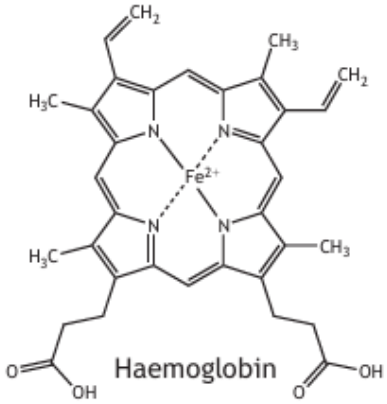
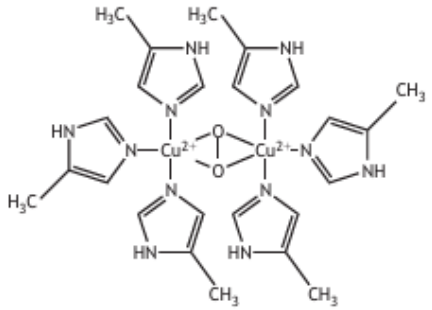
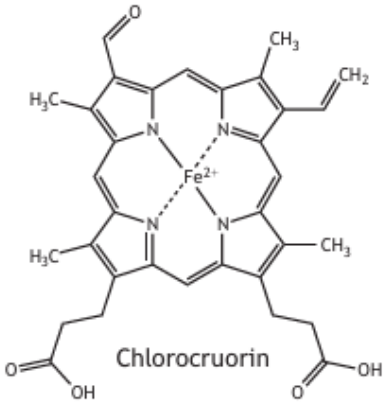
(i) Explain why methanol is a suitable solvent for this extraction. **1**

both polar/similar intermolecular forces

OR Forms hydrogen bonds with alizarin

Conjugation systems Past Papers

10.

Animal	Complex ion	Colour of blood
 Human	 Haemoglobin	RED
 Spider	 Oxyhaemocyanin	BLUE
 Leech	 Chlorocruorin	GREEN

Using your knowledge of chemistry, comment on why these animals have different coloured blood. **3**

All blood pigments have **large conjugated systems (alternating single and double bond chains)** which result in relatively lower energy gaps between HOMO and LUMO so they absorb visible light and appear coloured rather than absorbing higher energy UV light and appearing colourless.

The spider's oxyhaemocyanin has the largest conjugation system resulting in the lowest energy gap between HOMO and LUMO. To promote electrons. lower energy/frequency aka higher wavelength red and green (yellow) light is absorbed (580nm). The complementary colour (blue) is emitted and this is the colour of the blood.

The leech 's chlorocruorin has the smallest conjugation system resulting in the highest energy gap between HOMO and LUMO . To promote electrons, the highest energy/frequency aka lowest wavelength red & blue light is absorbed (purple 380nm). The complementary colour green is then emitted and is the colour of the blood.

The human's haemoglobin has a conjugation system size in between the larger spider and smaller leech .This results in an intermediate sized energy gap between HOMO & LUMO requiring intermediate size visible energy to be absorbed. Thus blue/green wavelengths (intermediate energy/frequency & intermediate wavelength of 500nm) is absorbed. The complementary colour red is then emitted and is the colour of the blood.