WJEC (Wales) Chemistry A-level

Topic 4.2 - Aromaticity

Flashcards

Give the molecular and skeletal formula of benzene

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Molecular formula: C_6H_6

Skeletal formula:

How can the structure of benzene be represented? Which model is more suitable?

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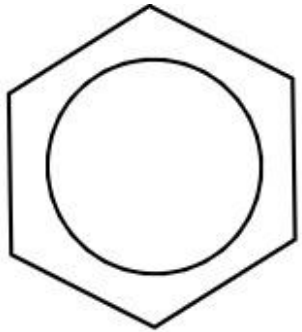

The first model is more suitable because the second model does not demonstrate the delocalised electron system.

Describe the bonding in benzene

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Benzene has six carbon atoms which each form a single covalent bond to the carbons next to it and to a hydrogen atom. This means each carbon atom has one unpaired electron in the outer p-orbital. These unpaired electrons combine to form a delocalised ring of electrons.

Explain the delocalised electron system of benzene in terms of the types of bonds involved

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The p orbital on each carbon atom in benzene overlaps with the p orbitals either side of them. This series of overlaps produces a pi bond system. These electrons are spread out over the whole carbon ring and therefore are described as being delocalised.

What is the shape and bond angle of benzene?

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Benzene is a planar, regular hexagon and the shape around each carbon atom is trigonal planar. The bond angle is 120º.

What is the general name for compounds containing a benzene ring?

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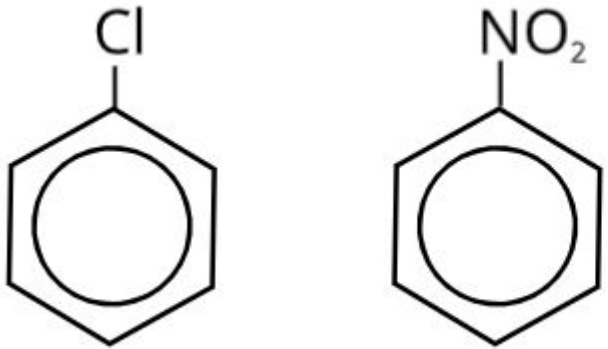
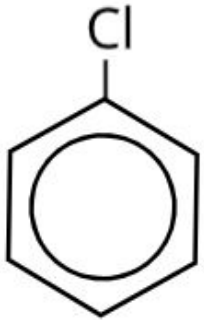
Arenes or aromatic compounds.

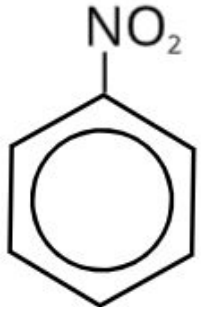
Name the following arenes



Name the following arenes

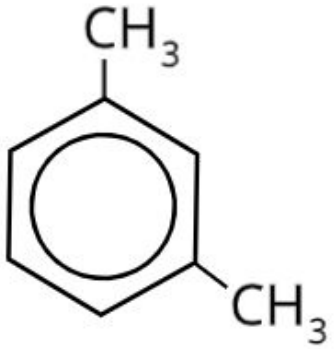


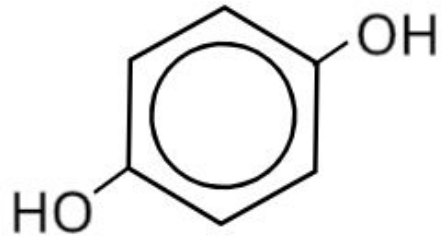
Chlorobenzene



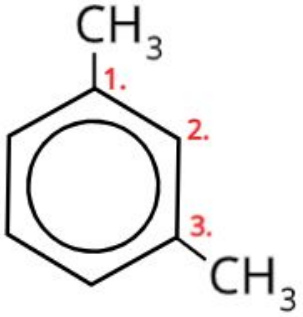
Nitrobenzene

Name the following arenes

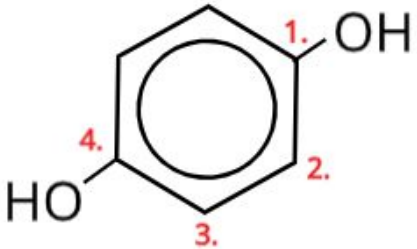




Name the following arenes



1,3-dimethylbenzene



Benzene-1,4-diol

Why does benzene not undergo electrophilic addition reactions?

Why does benzene not undergo electrophilic addition reactions?

Benzene's delocalised ring of electrons is a region of high electron density which attracts electrophiles. However, the ring of electrons is very stable so benzene does not undergo electrophilic addition as this would break up the delocalised ring of electrons.

What are the two common electrophilic substitution mechanisms for benzene?

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Friedel-Crafts acylation

Nitration reaction

How is the acyl chloride electrophile made stronger for Friedel-Crafts acylation?

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An acyl chloride is reacted with $AlCl_3$. The $AlCl_3$ accepts a lone pair of electrons from the acyl chloride. This increases the polarisation in the acyl chloride and it forms a carbocation. This is a much stronger electrophile so it is able to react with the benzene ring.

Give the equation for the reaction between aluminium chloride and ethanoyl chloride

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$$CH_3COCl + AlCl_3 \rightarrow CH_3C^+O + AlCl_4^-$$

Draw the electrophilic substitution mechanism for the reaction between benzene and methanoyl chloride

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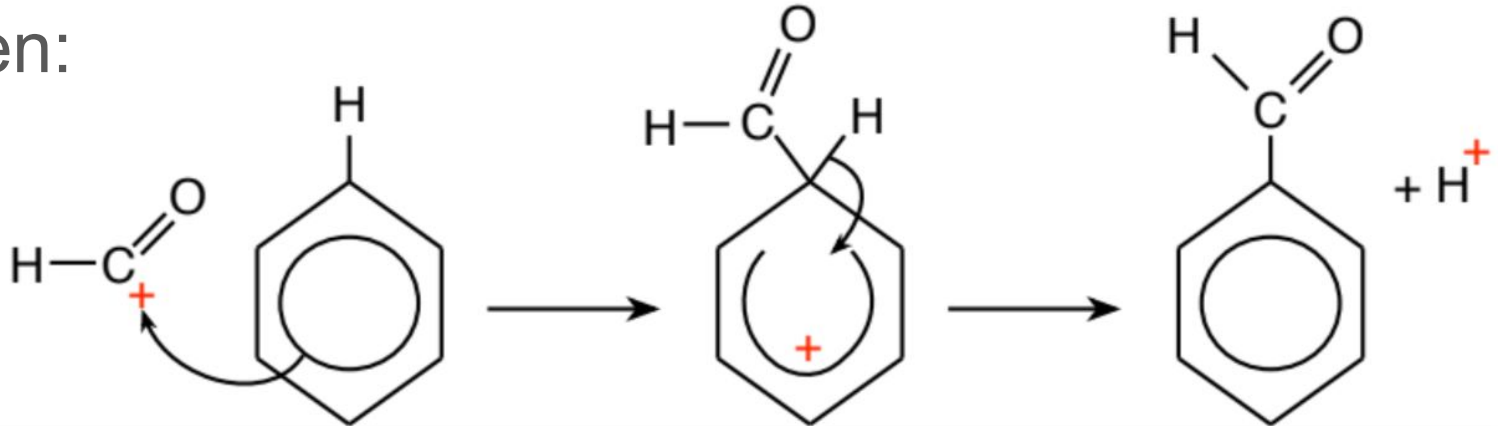
Initially: $HCOCl + AlCl_3 \rightarrow HC^{+}O + AlCl_4^{-}$

Then:



Explain how $AlCl_3$ behaves as a catalyst in the Friedel-Crafts acylation of benzene

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$AlCl_3$ initially reacts with an acyl chloride to produce a reactive carbocation intermediate and $AlCl_4^-$. At the end of the mechanism a hydrogen ion is released from the benzene ring. This reacts with the $AlCl_4^-$ to produce HCl and $AlCl_3$. Therefore $AlCl_3$ does not get used up during the reaction and so acts as a catalyst.

What conditions are required for Friedel-Crafts acylation reactions?

What conditions are required for Friedel-Crafts acylation reactions?

The reactants should be heated under reflux in a non-aqueous solvent.

Why are electrophiles attracted to benzene?

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Electrophiles are electron pair acceptors so are attracted to areas of high electron density. Benzene has a ring of delocalised electrons. This is an area of high electron density so it attracts electrophiles.

Give the reactants and catalyst required for the nitration of benzene

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Reactants: Benzene

Concentrated nitric acid

Catalyst: Concentrated sulfuric acid

How is the electrophile, NO_2^+, produced for the nitration of benzene?

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Concentrated nitric and sulfuric acid react to form the NO_2^+ intermediate:

$$HNO_3 + H_2SO_4 \rightarrow H_2NO_3^+ + HSO_4^-$$

$$H_2NO_3^+ \rightarrow NO_2^+ + H_2O$$

Draw the electrophilic substitution mechanism for the nitration of benzene

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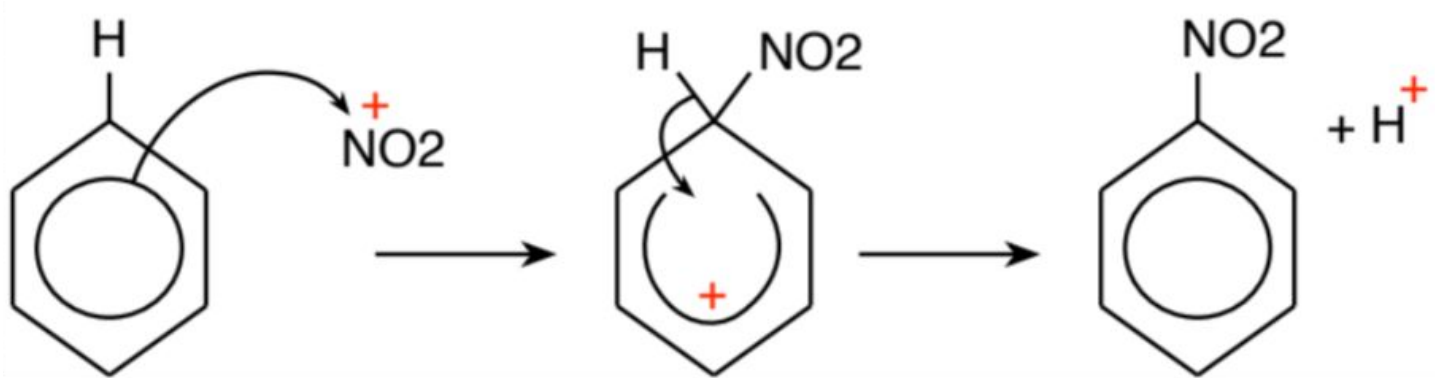

How does sulfuric acid act as a catalyst in the nitration of benzene?

How does sulfuric acid act as a catalyst in the nitration of benzene?

Initially sulfuric acid reacts to produce the NO_2^+ electrophile:

$HNO_3 + H_2SO_4 \rightarrow H_2NO_3^+ + HSO_4^-$ $\quad\quad$ $H_2NO_3^+ \rightarrow NO_2^+ + H_2O$

At the end of the mechanism a hydrogen ion is released from benzene. This reacts with the HSO_4^- ion to reproduce H_2SO_4. Therefore H_2SO_4 does not get used up and so acts as a catalyst.

What condition ensures mononitration will occur in the nitration of benzene?

What condition ensures mononitration will occur in the nitration of benzene?

Mononitration is when only one NO_2 group is added to benzene. This occurs if the temperature is kept below 55°C.

Draw the electrophilic substitution mechanism for the reaction between benzene and chlorine

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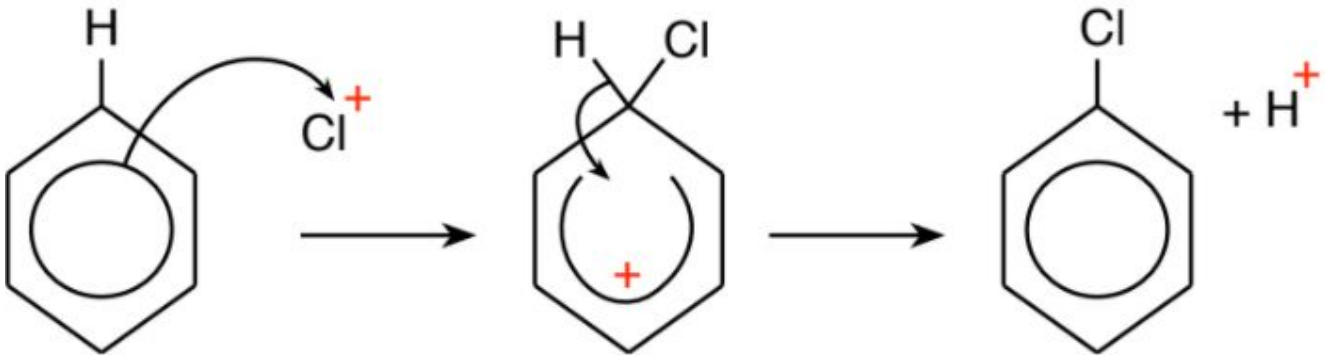

Why is the C-Cl bond stronger in benzene than in a chloroalkane?

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The lone pair of electrons on the chlorine atom is delocalised over the benzene ring which strengthens the carbon-chlorine bond.

Why is chlorobenzene unreactive towards nucleophiles?

Why is chlorobenzene unreactive towards nucleophiles?

The C-Cl bond in benzene is stronger than in halogenoalkanes. This makes it harder to break and so is not easily attacked by nucleophiles.