

### AQA Chemistry A-level

Topic 3.10 - Aromatic Chemistry

**Flashcards** 

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### What is benzene's formula and structure?



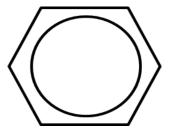








#### What is benzene's formula and structure?











## What is another name for arenes? Why did this come about?











What is another name for arenes? Why did this come about?

Aromatic compounds, as first found in sweet-smelling dyes











### What is the most common type of reaction of benzene?











What is the most common type of reaction of benzene?

Substitution (of a H for a different functional group)









### What is the shape of benzene?













What is the shape of benzene?

Flat, regular hexagon. Bond angle = 120°









### What is the bond length between adjacent C atoms?











What is the bond length between adjacent C atoms?

Intermediate between C-C and C=C











What happens to the 4th electron in the p orbital of each C atom in benzene?













What happens to the 4th electron in the p orbital of each C atom in benzene?

It delocalises to form rings of electron density above and below the hexagon, forming rings of delocalised electron density above/below the hexagon.









What is the effect on benzene's stability of the rings of electron density?









What is the effect on benzene's stability of the rings of electron density?

Makes benzene very stable, even though it is unsaturated (aromatic stability)







### Draw the skeletal structure of cyclohexa-1,3,5-triene



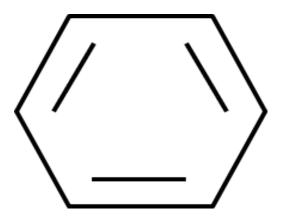








#### Draw the skeletal structure of cyclohexa-1,3,5-triene













What is the thermochemical evidence that benzene is more stable than cyclohexa-1,3,5-triene?









What is the thermochemical evidence that benzene is more stable than cyclohexa-1,3,5-triene?

Hydrogenation of cyclohexene = -120kJmol<sup>-1</sup> →

cyclohexa-1,3,5-triene = -360kJmol<sup>-1</sup>

Benzene hydrogenation = -208kJmol<sup>-1</sup> so benzene is 152kJmol<sup>-1</sup> more stable







## Why else is cyclohexa-1,3,5-triene not a suitable model for benzene?













#### Why else is cyclohexa-1,3,5-triene not a suitable model for benzene?

Would not be symmetrical (C=C shorter than C-C), but benzene is

Would easily undergo addition reactions across the double bonds - benzene does not

Would form two isomers on the addition of Br<sub>2</sub> or similar benzene does not









### What is the appearance of benzene at 298K?











What is the appearance of benzene at 298K?

#### Colourless liquid









## Why does benzene have a relatively high melting point?











Why does benzene have a relatively high melting point?

Close packing of flat hexagonal molecules when solid









### Is benzene soluble in water? Why?











Is benzene soluble in water? Why?

No- non polar













# Dangers of benzene? (why it is not used in schools)











Dangers of benzene? (why it is not used in schools)

It is a carcinogen











# How do you name compounds containing a benzene ring?











How do you name compounds containing a benzene ring?

-benzene, or phenyl-; can designate position on ring using numbers if there is more than one substituent









### Why is benzene attacked by electrophiles?











Why is benzene attacked by electrophiles?

High electron density above/below ring due to delocalised electrons









# What is delocalisation energy and what is the effect of this on benzene's reactions?









What is delocalisation energy and what is the effect of this on benzene's reactions?

The large amount of energy that is needed to break the aromatic ring apart. Results in the aromatic ring almost always staying intact









### What is seen when benzene is combusted? Why?











What is seen when benzene is combusted? Why?

Smoky flames due to soot from unburnt carbon.

This is because of the high Carbon: Hydrogen ratio.









Draw a general electrophilic substitution mechanism of benzene, using EI<sup>+</sup> to represent an electrophile.

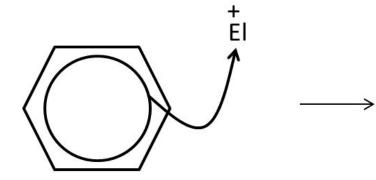


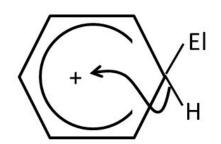






Draw a general electrophilic substitution mechanism of benzene, using EI<sup>+</sup> to represent an electrophile













## Which ion (name and formula) is used to nitrate benzene?











Which ion (name and formula) is used to nitrate benzene?

NO<sub>2</sub><sup>+</sup> (+ charge is on the nitrogen). Nitronium ion or nitryl cation







## How is this NO<sub>2</sub><sup>+</sup> ion generated? (conditions and equations)











How is this NO<sub>2</sub><sup>+</sup> ion generated? (conditions and equations)

Concentrated H<sub>2</sub>SO<sub>4</sub> and concentrated HNO<sub>3</sub>.

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

$$H_2NO_3^+ \to H_2O + NO_2^+$$

Overall: 
$$H_2SO_4 + HNO_3 \rightarrow HSO_4^- + NO_2^+ + H_2O_3^-$$







## How is the H<sub>2</sub>SO<sub>4</sub> catalyst regenerated in the nitration of benzene?











How is the H<sub>2</sub>SO<sub>4</sub> catalyst regenerated in the nitration of benzene?

 $HSO_{4}^{-} + H^{+} \rightarrow H_{2}SO_{4}$  (H<sup>+</sup> from benzene ring)









# Draw a mechanism and write an overall equation for the nitration of benzene





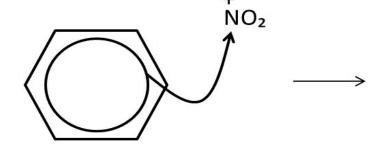


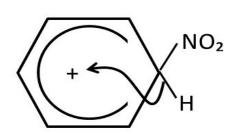




Draw a mechanism and write an overall equation for the nitration of benzene

$$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O_3$$















#### What are the uses of nitrated arenes?











What are the uses of nitrated arenes?

Production of explosives e.g. TNT

(1-methyl-2,4,6-trinitrobenzene) - releases lots of

heat and gas on explosion.

To make aromatic amines that are used for industrial dyes









How do substituents with a positive inductive effect (e.g. alkyl groups) affect further substitution?









How do substituents with a positive inductive effect (e.g. alkyl groups) affect further substitution?

They release electrons into the delocalised electron ring, increasing the electron density and making further substitution reactions more likely/quick.

Direct substituents to the 2,4,6 positions









How do substituents with a negative inductive effect (e.g. NH<sub>2</sub>) affect further substitution?









How do substituents with a negative inductive effect (e.g. NH<sub>2</sub>) affect further substitution?

Remove electrons from the delocalised electron ring, decreasing the electron density and making further substitution reactions less likely/quick.

Direct substituents to 3,5 positions









# What type of catalyst is used for a Friedel-Crafts reaction?











What type of catalyst is used for a Friedel-Crafts reaction?

A halogen carrier (e.g. AlCl<sub>3</sub>)









Write an equation to form an electrophile that could be used to acylate benzene, starting with AICI, and RCOCI









Write an equation to form an electrophile that could be used to acylate benzene, starting with AICI3 and **RCOCI** 

$$AICI_3 + RCOCI \rightarrow AICI_4^- + RCO^+ (+ on C)$$

RCO<sup>+</sup> can attack benzene









## What is happening when AICI, is formed in terms of electrons?









What is happening when AlCl<sub>4</sub> is formed in terms of electrons?

Chlorine atom's lone pair of electrons is forming a coordinate bond to Al







### How is the AICI<sub>3</sub> catalyst reformed?











#### How is the AlCl<sub>3</sub> catalyst reformed?

$$AICI_4^- + H^+ \rightarrow HCI + AICI_3 (H^+ from benzene)$$









## How could you use a Friedel-Crafts mechanism to add a methyl group to a benzene ring?









How could you use a Friedel-Crafts mechanism to add a methyl group to a benzene ring?

Use a halogenoalkane and AICI<sub>3</sub> to create an electrophile that can attack benzene









## Draw the mechanism for the acylation of benzene from RCO<sup>+</sup>.





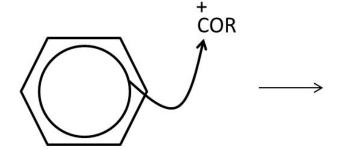


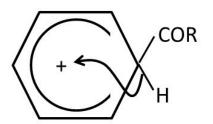






Draw the mechanism for the acylation of benzene from RCO<sup>+</sup>.













If you are considering cyclic compounds, what might happen if two double bonds are next to each other?









If you are considering cyclic compounds, what might happen if two double bonds are next to each other?

C=C bonds are in close proximity, so electrons in pi cloud/p orbitals can partially delocalise and move between the two C=C double bonds









What effect would electrons in p orbitals moving between the two C=C double bonds have on the stability of the molecule and its enthalpy of hydrogenation?









What effect would electrons in p orbitals moving between the two C=C double bonds have on the stability of the molecule and its enthalpy of hydrogenation?

Makes the molecule more stable; makes enthalpy of hydrogenation more positive



