

## 5.3.1 Use benzene evidence and select substitution conditions

Name: \_\_\_\_\_ Class: \_\_\_\_\_ Date: \_\_\_\_\_

Total: 18 marks

**KEY WORDS** evidence • conditions

### Objective

Use benzene evidence and select substitution conditions. All questions and marking guidance are original.

### 1 Key knowledge and worked examples

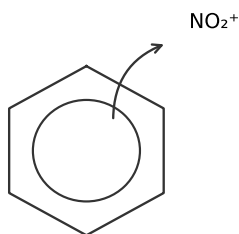
Benzene has equal C–C lengths and a delocalised ring. Addition would destroy that system. Electrophilic substitution replaces H then restores delocalisation. Phenol reacts with bromine water more readily because oxygen's lone pair increases ring electron density.

#### ■ Worked method

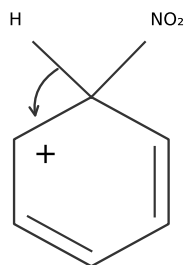
If three isolated C=C bonds predict hydrogenation  $-360 \text{ kJ mol}^{-1}$  but benzene gives  $-208$ , benzene is  $152 \text{ kJ mol}^{-1}$  more stable than that hypothetical localised model. Nitration uses concentrated  $\text{HNO}_3/\text{H}_2\text{SO}_4$ .  $\text{HNO}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{NO}_2^+ + \text{HSO}_4^- + \text{H}_2\text{O}$  generates the electrophile. A ring electron pair attacks  $\text{NO}_2^+$ ; loss of  $\text{H}^+$  restores the ring.

Nitration mechanism after  $\text{NO}_2^+$  generation; curly arrows show electron pairs

1 Ring electron pair attacks

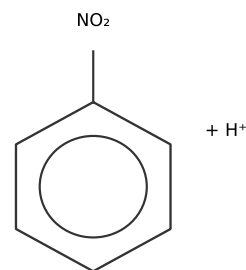


2 Positive intermediate



C–H bond pair restores ring

3 Nitrobenzene +  $\text{H}^+$



## 2 Practice

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**2.1** Give two pieces of evidence against three separate ordinary C=C bonds in benzene. [2]

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**2.2** Calculate stabilisation relative to the hypothetical model if one C=C hydrogenation is  $-118 \text{ kJ mol}^{-1}$  and benzene is  $-206 \text{ kJ mol}^{-1}$ . [3]

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**2.3** State benzene bromination conditions and compare phenol with bromine water. [3]

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## 3 Exam-style questions

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**3.1** Write the nitrating-electrophile generation equation and name the electrophile. Explain how substitution retains the aromatic system overall. [4]

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**3.2** Give reagents for making ethylbenzene and phenylethanone from benzene. Identify which is Friedel–Crafts acylation. [3]

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**3.3** A student predicts benzene will rapidly decolourise bromine water because it has six  $\pi$  electrons. Explain the error, and state sulfonation conditions. [3]

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