

# 29.3 Shape and bonding of benzene

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

Total: 21 marks

**KEY WORDS** delocalised 离域 • benzene 苯 • hybridisation 杂化  
• enthalpy change of hydrogenation 氢化焓变

## Objective

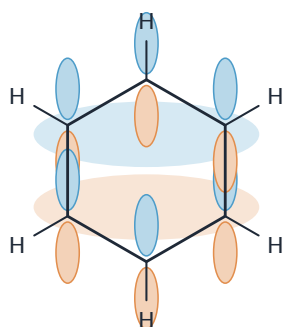
Build the skills to answer exam questions on the **shape and bonding of benzene** 苯的形状与成键 —  $\text{sp}^2$  hybridisation,  $\sigma$  and  $\pi$  bonds, **delocalisation** 离域, and the evidence for it.

**You must be able to:**

- describe benzene as a planar regular hexagon of  $\text{sp}^2$  carbons
- explain the  $\sigma$  framework and the delocalised  $\pi$  system
- use enthalpy of hydrogenation as evidence for delocalisation

## 1 Worked examples

### ■ Bonding and stability



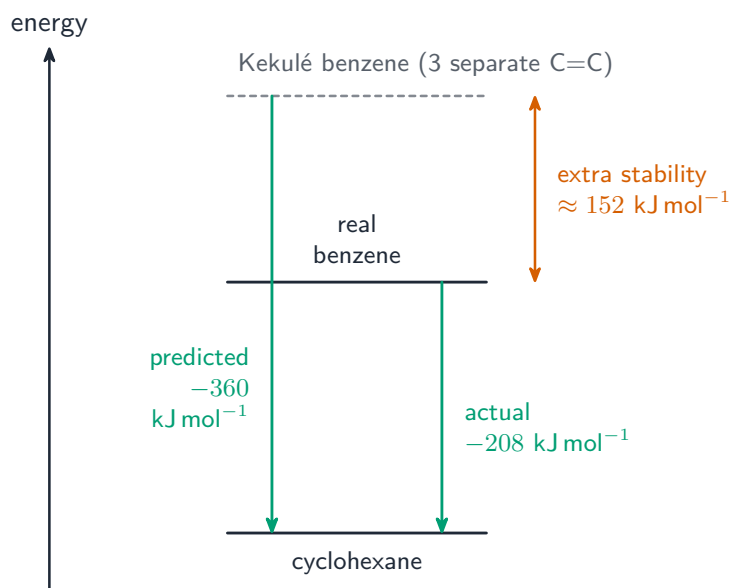
one **delocalised**  $\pi$  system  
above and below the ring

$\text{sp}^2$   $\sigma$  framework;  
all six C-C bonds equal

*Each carbon is  $\text{sp}^2$ : three  $\sigma$  bonds make the flat hexagon; the leftover p orbitals overlap into one delocalised  $\pi$  system*

- each C is  $\text{sp}^2$ : three  $\sigma$  bonds (to 2 C + 1 H) in the plane.
- each C keeps one electron in a **p orbital**; these overlap sideways all round → one **delocalised**  $\pi$  ring above and below the plane.
- all six C-C bonds are **equal length** (between single and double); the ring is very stable.

## ■ Evidence: enthalpy of hydrogenation



*Real benzene releases only 208 kJ mol<sup>-1</sup> vs the Kekulé prediction 360 = 3 × cyclohexene → ~152 more stable*

The shortfall ( $360 - 208 = 152 \text{ kJ mol}^{-1}$ ) is the extra stability from delocalisation.

## 2 Practice

2.1 State the hybridisation of each carbon atom in benzene.

[1]

2.2 State what the equal C–C bond lengths in benzene tell you about its bonding.

[1]

## 3 Exam-style questions

3.1 The  $\pi$  system in benzene is formed by the overlap of:

[1]

|   |   |
|---|---|
| A | B |
| C | D |

A  $\text{sp}^2$  hybrid orbitals

B s orbitals

C p orbitals at right angles to the ring

D  $\text{sp}^3$  hybrid orbitals

**3.2** Hydrogenation of cyclohexene releases  $120 \text{ kJ mol}^{-1}$ . The Kekulé model of benzene would predict a hydrogenation enthalpy of about: [1]

|   |   |
|---|---|
| A | B |
| C | D |

**A**  $-120 \text{ kJ mol}^{-1}$

**B**  $-208 \text{ kJ mol}^{-1}$

**C**  $-240 \text{ kJ mol}^{-1}$

**D**  $-360 \text{ kJ mol}^{-1}$

**3.3** Describe the bonding in benzene, referring to  $\text{sp}^2$  hybridisation, the  $\sigma$  framework and the delocalised  $\pi$  system. [3]

---

---

---

**3.4** The real enthalpy of hydrogenation of benzene is  $-208 \text{ kJ mol}^{-1}$ ; the Kekulé prediction is  $-360 \text{ kJ mol}^{-1}$ . State and explain what this difference shows. [2]

---

---

**3.5** Benzene is a planar molecule with all six C–C bonds of the same length, 0.139 nm. (C–C in ethane is 0.154 nm; C=C in ethene is 0.134 nm.)

(a) Describe the bonding in benzene in terms of  $sp^2$  hybridisation,  $\sigma$  bonds and  $\pi$  bonds.[4]

---

---

---

---

---

(b) Explain how the bond-length data support the delocalised model rather than the Kekulé structure. [2]

---

---

(c) The enthalpy change of hydrogenation of cyclohexene is  $-120 \text{ kJ mol}^{-1}$ , and of benzene  $-208 \text{ kJ mol}^{-1}$ . Explain what these values show, with a calculation. [3]

---

---

---

---

(d) Explain why benzene undergoes substitution rather than addition. [3]

---

---

---