29.3 Shape and bonding of benzene

Name: ______________ Class: __________ Date: ____________ **Total: 9 marks**

Objective

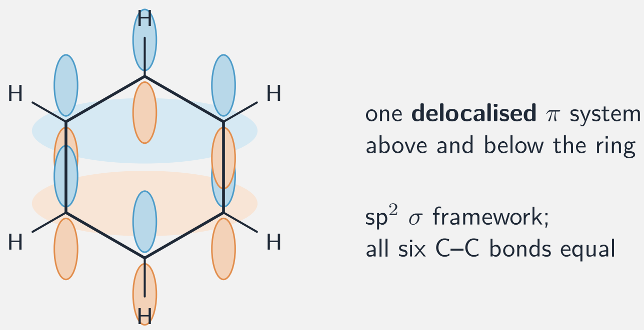
Build the skills to answer exam questions on the **shape and bonding of benzene 苯的形状与成键**—**sp²** hybridisation, σ and π bonds, **delocalisation 离域**, and the evidence for it.

You must be able to:

- describe benzene as a planar regular hexagon of sp^2 carbons
- explain the σ framework and the delocalised π system
- use enthalpy of hydrogenation as evidence for delocalisation

1 Worked examples

Bonding and stability



Each carbon is sp²: three σ bonds make the flat hexagon; the leftover p orbitals overlap into one delocalised π system

- each C is **sp²**: three σ 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** π ring above and below the plane.
- all six C–C bonds are **equal length** (between single and double); the ring is very stable.

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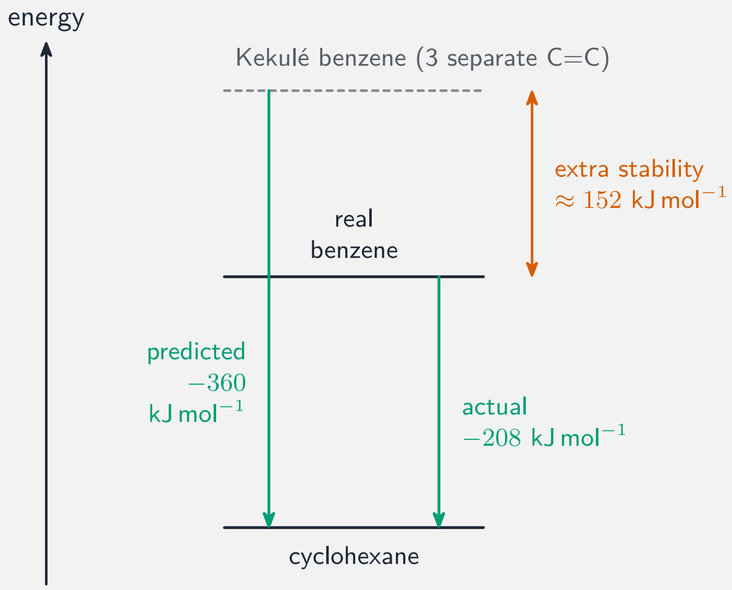

Real benzene releases only 208 $kJ\,mol^{-1}$ vs the Kekulé prediction $360 = 3\times$ cyclohexene → ~152 more stable

The shortfall ($360 - 208 = 152$ 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 π system in benzene is formed by the overlap of: [1]

- **A** sp^2 hybrid orbitals
- **B** s orbitals
- **C** p orbitals at right angles to the ring
- **D** sp^3 hybrid orbitals

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

- **A** $-120\ \mathrm{kJ\,mol^{-1}}$
- **B** $-208\ \mathrm{kJ\,mol^{-1}}$
- **C** $-240\ \mathrm{kJ\,mol^{-1}}$
- **D** $-360\ \mathrm{kJ\,mol^{-1}}$

3.3 Describe the bonding in benzene, referring to sp^2 hybridisation, the σ framework and the delocalised π system. [3]

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

4 Go further

You are now ready for the real exam questions on this subtopic. Open the **29.3 Shape and bonding of benzene** past-paper sheet in the Library, or try these in **Practice mode**:

- 9701/42 N25 —Q9 (shape and bonding of benzene)
- 9701/44 N25 —Q5 (shape and bonding of benzene)
- 9701/44 N25 —Q6 (shape and bonding of benzene)

Solutions

2.1 sp^2.

2.2 the bonding is delocalised / identical round the ring (not alternating single and double bonds).

3.1 C. The p orbitals at right angles to the ring overlap sideways to form the delocalised π system.

3.2 D. Three C=C $\times$ 120 = -360 kJ mol^{-1}.

3.3 each carbon is sp^2 hybridised, forming three σ bonds (to two C and one H) in a planar hexagon; each carbon has one electron in a p orbital perpendicular to the ring; these p orbitals overlap sideways all round to give one delocalised π system above and below the plane.

3.4 benzene is about 152 kJ mol^{-1} more stable than the Kekulé model predicts; this extra stability is due to delocalisation of the π electrons.