

29.3 Shape and bonding of benzene

Name: _____ Class: _____ Date: _____

Total: 9 marks

KEY WORDS delocalised 离域 • benzene 苯 • hybridisation 杂化

Objective

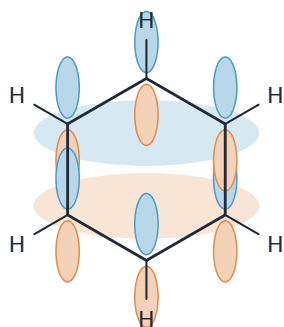
Build the skills to answer exam questions on the **shape and bonding of benzene** 苯的形状与成键 — sp^2 hybridisation, σ and π bonds, **delocalisation** 离域, and the evidence for it.

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



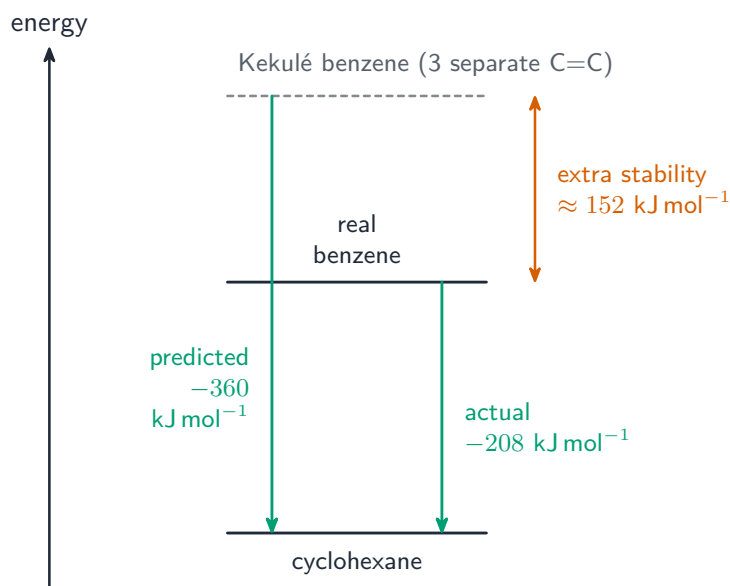
one **delocalised** π system
above and below the ring

sp^2 σ framework;
all six C-C bonds equal

Each carbon is sp^2 : three σ bonds make the flat hexagon; the leftover p orbitals overlap into one delocalised π system

- each C is sp^2 : 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.

■ Evidence: enthalpy of hydrogenation



Real benzene releases only 208 kJ mol⁻¹ 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 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 kJ mol^{-1}
 - **B** -208 kJ mol^{-1}
 - **C** -240 kJ mol^{-1}
 - **D** -360 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 kJ mol^{-1} ; the Kekulé prediction is -360 kJ mol^{-1} . State and explain what this difference shows.

[2]

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 $\text{C}=\text{C} \times 120 = -360 \text{ kJ mol}^{-1}$.

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.