Exercise walk-through

Shapes of aromatic organic molecules; σ and π bonds ▪ 29.3

eXercise

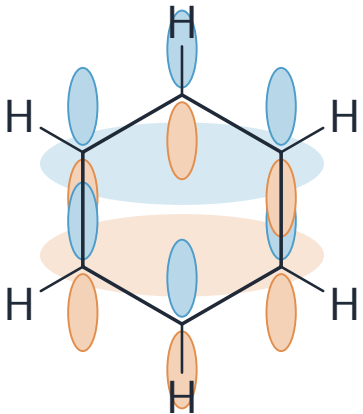
You must be able to

- 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

Method — Bonding and stability

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 $\rightarrow$ 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.



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

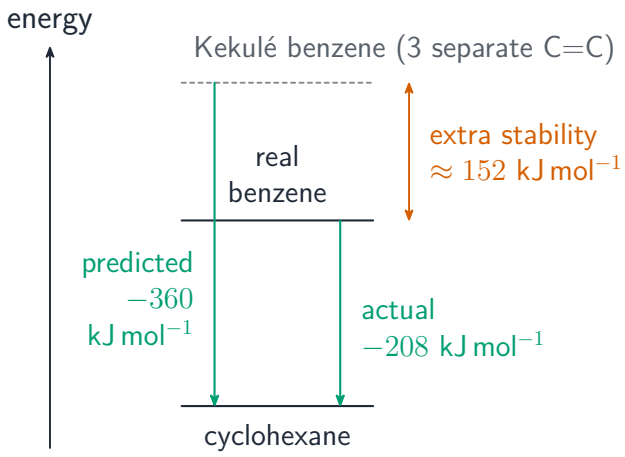
sp^2 σ framework;
all six C–C bonds equal

Method — Evidence: enthalpy of hydrogenation

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

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

Method — Evidence: enthalpy of hydrogenation



Practice 2.1 ▪ 1 mark

State the hybridisation of each carbon atom in benzene.

Solution 2.1

Method: Bonding and stability

Worked steps

sp^2 B1.

Practice 2.2 ▪ 1 mark

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

Solution 2.2

Method: Bonding and stability

Worked steps

the bonding is delocalised / identical round the ring (not alternating single and double bonds) **B1**.

Exam-style 3.1 ▪ 1 mark

The π system in benzene is formed by the overlap of:

A sp^2 hybrid orbitals

B s orbitals

C p orbitals at right angles to the ring

D sp^3 hybrid orbitals

Solution 3.1

Method: Bonding and stability

A sp^2 hybrid orbitals

B s orbitals

C p orbitals at right angles to the ring ✓

D sp^3 hybrid orbitals

Worked steps

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

Exam-style 3.2 ▪ 1 mark

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

A -120 kJ mol^{-1}

B -208 kJ mol^{-1}

C -240 kJ mol^{-1}

D -360 kJ mol^{-1}

Solution 3.2

Method: Evidence: enthalpy of hydrogenation

A -120 kJ mol^{-1}

B -208 kJ mol^{-1}

C -240 kJ mol^{-1}

D -360 kJ mol^{-1} ✓

Worked steps

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

Exam-style 3.3 ▪ 3 marks

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

Solution 3.3

Method: Bonding and stability

Worked steps

each carbon is sp^2 hybridised, forming three σ bonds (to two C and one H) in a planar hexagon **M1**; each carbon has one electron in a p orbital perpendicular to the ring **M1**; these p orbitals overlap sideways all round to give one delocalised π system above and below the plane **A1**.

Exam-style 3.4 ▪ 2 marks

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.

Solution 3.4

Method: Evidence: enthalpy of hydrogenation

Worked steps

benzene is about 152 kJ mol^{-1} more stable than the Kekulé model predicts **M1**; this extra stability is due to delocalisation of the π electrons **A1**.