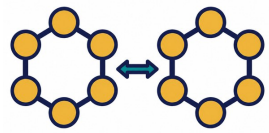
Benzene Structure Map

OCR A Level Chemistry A · 6.1.1 Benzene structure and stability

1 Two models

6.1.1(a)

- C_6H_6: one H on each carbon
- Kekulé: **alternating** C=C and C–C
- Cyclohexa-1,3,5-triene
- Delocalised: **six equal bonds**



2 Bonding

6.1.1(a)

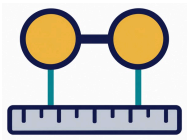
- Each C: three σ-bonds, planar, 120°
- One **p-orbital** per carbon
- p-orbitals **overlap sideways**
- π-system above and below the ring

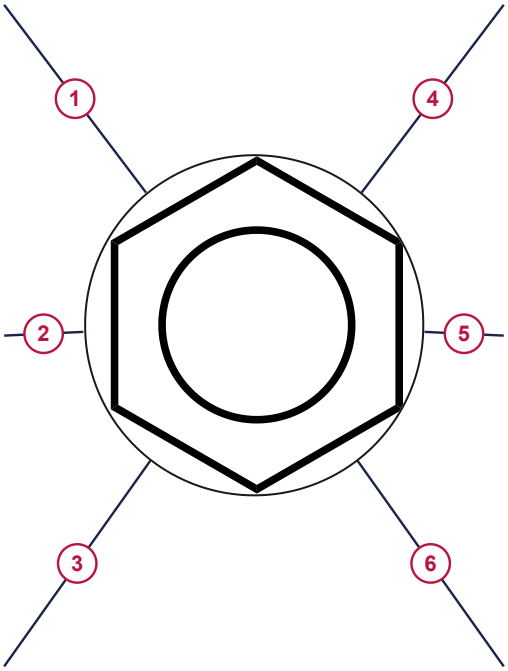


3 Bond lengths

6.1.1(b)

- C–C 0.154 nm; C=C 0.134 nm
- Benzene: all six **0.139 nm**
- **Between** single and double
- So not alternating

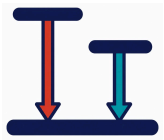




4 Hydrogenation

6.1.1(b)

- Cyclohexene −120 kJ mol^{-1}
- Kekulé predicts **−360**
- Benzene measured **−208**
- **152 kJ mol^{-1} more stable**



5 Resistance to bromine

6.1.1(f)

- Cyclohexene: orange to colourless
- Benzene: **no reaction**
- Alkene: localised, polarises Br_2
- Benzene: delocalised, **lower density**



6 Naming

6.1.1(c)

- Methylbenzene, nitrobenzene
- New parent: **phenol, benzoic acid**
- **Lowest numbers** round the ring
- Prefixes in **alphabetical order**



Kekulé against the evidence

what each model predicts and what is found

Test	Kekulé predicts	Found
Ring bond lengths	Two	One, 0.139 nm
ΔH hydrogenation	−360 kJ mol^{-1}	−208 kJ mol^{-1}
Bromine water	Decolourises	No reaction
Dibromobenzenes	Four	Three

Worked examples

Formula

- 92.3% C, Mr 78
- C:H = 1:1, so CH
- **78 ÷ 13 = 6: C_6H_6**

Stability

- 3 × −120 = −360
- −360 against −208
- **152 kJ mol^{-1}**

Naming

- Cl opposite CH_3
- Alphabetical: chloro first
- **1-chloro-4-methylbenzene**

Electrophilic substitution, phenol and directing effects follow in the next section of 6.1.1.

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