simplest arene ~ # BENZENE

C_6H_6

Q: Why ⬡(—) not accurate
· All C to C bonds same length
Explain diff arrange^n e$^-$:
· π / 6 e$^-$ of C =deloc in benzene

· **aliphatic** : straight/branched chain org subs
· **aromatic** : have planar, unsat. ring (pleasent smell)
· **arene** : ≳1 ring 6 C atoms w̄ delocalised bonding
  ↳ = aromatic hydrocarbon

STRUCTURE

· C_6H_6
  ↳ 6 C atoms hex·ring (one H bonded each C)
· = planar mol

(· e$^-$ deloc around ring ; overlap p-orbitals)

Actual struct: ⬡(◯) ✓
  ↳ deloc e$^-$ system

H–C–C bond angle = 120°

Kekulé model ~ evidence to prove **WRONG**

displayed formula   skeletal formula

✗
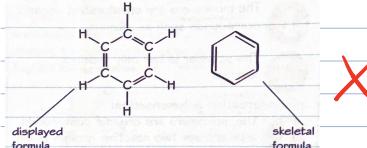
*benz ring = large, non polar
&hydrophobic

delocalised model:
· 6 p e$^-$ =deloc in ring above + below
  ρ   plane Carbon ring.
· 6 orbitals overlap → 3 π bonds
  π bonds ~ clouds deloc· e$^-$
· e$^-$ constant move (shared equally bet 6 C atoms)
 → **Stability**
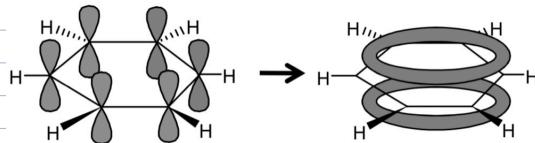
EVIDENCE AGAINST KEKULÉ

1. x decol^n Br_2 water (lack reactivity of benzene) - as not normal alkene

2. Thermodyn· stability ΔH hydrogenation   ⟵ver for benzene (than exp.)

⬡ + H_2 ⟶ ⬡ $\Delta H = -120 kJmol^{-1}$
cyclohexene
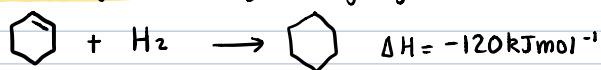
· delocalization ~ >stable of deloc π
· ∴ > E req break bonds in benzene
  ↳ (>endo ∴ ↓ exo value)

↳ If kekulé correct, $\Delta H_r^{\ominus}$ benzene SHOULD be   3 × = -360
BUT **NOT** (is -208)
∴ benzene = >stable (by 152 $kJmol^{-1}$)
(6 π e$^-$ =deloc, not as 3 C=C)

→ · Benzene >stable by 152$_{kJmol}$
  · π bond e$^-$ =deloc
  · sub^n rxns (instead add^n)
  · maintains deloc syst
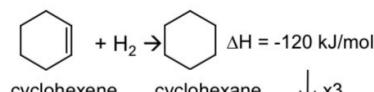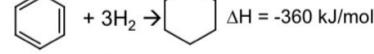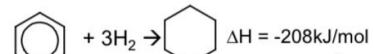
difference = delocalisation enthalpy

enthalpy
$\Delta H = -152kJ/mol$
delocalisation energy
-360 kJ/mol Theoretical value
$\Delta H = -208kJ/mol$ actual value

↳ ↓ exo than expected
due deloc stab ring from ring e$^-$

⬡ + H_2 → ⬡ $\Delta H = -120$ kJ/mol
cyclohexene   cyclohexane   ↓ x3
⬡ + $3H_2$ → ⬡ $\Delta H = -360$ kJ/mol
Non delocalised structure
⬡(◯) + $3H_2$ → ⬡ $\Delta H = -208kJ/mol$
delocalised structure