

# simplest arene $\rightarrow$ **BENZENE**



Q: Why not accurate  
 • All C to C bonds same length  
 Explain diff arrange<sup>n</sup>  $e^-$ :  
 •  $\pi/6$   $e^-$  of C = deloc in benzene

- **aliphatic**: straight/branched chain org sub
- **aromatic**: have planar, unsat. ring (pleasant smell)
- **arene**:  $\geq 1$  ring 6 C atoms w delocalized bonding  
 $\rightarrow$  = aromatic hydrocarbon

## STRUCTURE

- $C_6H_6$   
 $\rightarrow$  6 C atoms hex. ring (one H bonded each C)
- = **planar** mol  
 (•  $e^-$  deloc around ring; overlap p-orbitals)

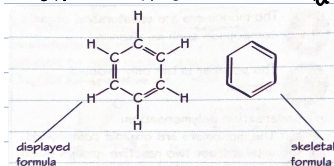
Actual struct:



$\rightarrow$  deloc  $e^-$  system

H-C-C bond angle =  $120^\circ$

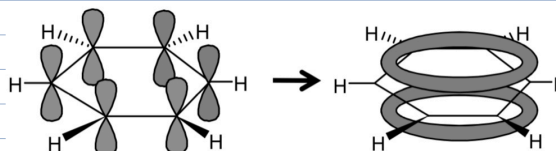
Kekulé model  $\rightarrow$  evidence to prove WRONG



benz ring = large, non polar & hydrophobic

delocalised model:

- 6 p  $e^-$  = deloc in ring above + below plane carbon ring.
- 6 p orbitals overlap  $\rightarrow$  3  $\pi$  bonds  
 $\pi$  bonds  $\rightarrow$  clouds deloc.  $e^-$
- $e^-$  constant move (shared equally bet 6 C atoms)  
 $\rightarrow$  **Stability**



## EVIDENCE AGAINST KEKULÉ

1. x decol<sup>n</sup> Br<sub>2</sub> water (lack reactivity of benzene) - as not normal alkene

2. Thermodyn. stability  $\Delta H$  hydrogenation



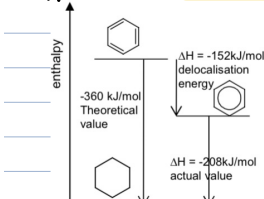
cyclohexene

$\rightarrow$  If Kekulé correct,  $\Delta H_f^\ominus$  benzene SHOULD be  $3 \times = -360$   
 BUT NOT (is -208)

$\therefore \rightarrow$  benzene = **> stable** (by  $152 \text{ kJ mol}^{-1}$ )  
 (6  $\pi e^-$  = deloc, not as 3 C=C)

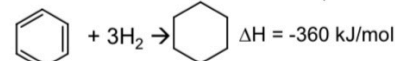
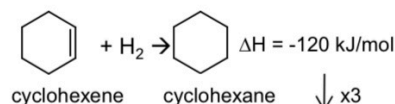
• delocalization  $\sim$  > stable of deloc  $\pi$   
 •  $\therefore$  > E req. break bonds in benzene  
 $\rightarrow$  (endo  $\therefore$   $\downarrow$  exo value)

difference = **delocalisation enthalpy**

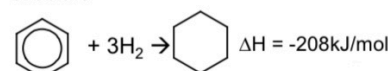


- Benzene > stable by  $152 \text{ kJ mol}^{-1}$
- $\pi$  bond  $e^-$  = deloc
- sub<sup>n</sup> rxns (instead add<sup>n</sup>)
- maintains deloc syst

$\rightarrow$   $\downarrow$  exo than expected  
 due deloc stablring from ring  $e^-$



Non delocalised structure



delocalised structure