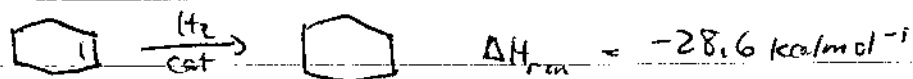


## Ch 16 Aromatic Compounds

Aromaticity - properties similar to benzene



$$\text{and } \Delta H_{\text{rxn}} = 3(-28.6 \text{ kcal mol}^{-1}) \\ = -85.8 \text{ kcal mol}^{-1}$$

However,



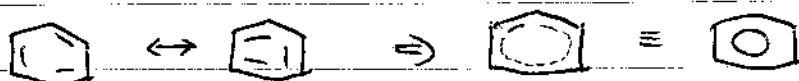
less exothermic rxn

WHY?

Stability from delocalization of  $\pi$ -electrons

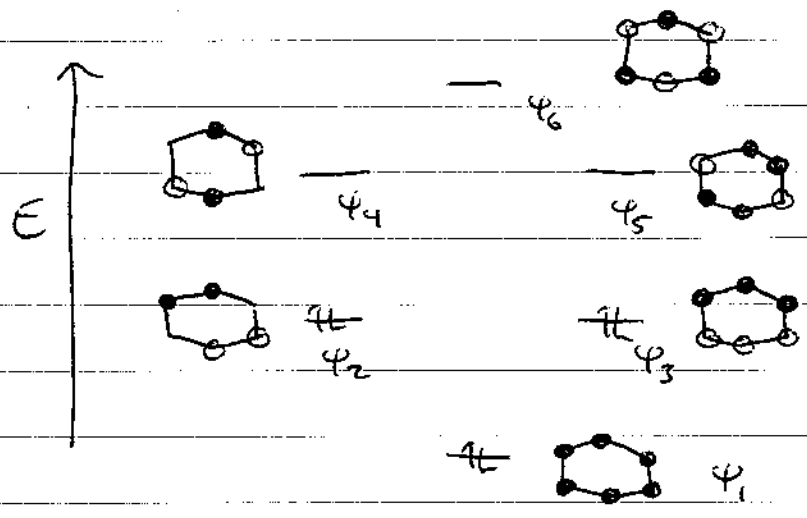
Called EMPIRICAL RESONANCE ENERGY

$$\Rightarrow \underline{36 \text{ kcal mol}^{-1}}$$



Aromatic Sextet 4n+2 Rule = Hückel Rule


Benzene - MO diagram





6  $\pi e^-$

Humm ... E. Hückel  $\rightarrow$  hey!  $4n+2$   
 $n = 0, 1, 2, 3, \dots$

Hückel Rule  $\Rightarrow$  For benzene  $4n+2 = 6$   $n = 1$

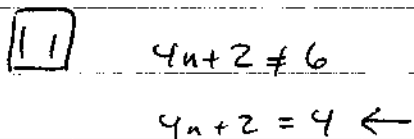
  
 $6\pi e^-$   
 also 1 p  
 non-bonding  
 (act as base)

  
 $6\pi e^-$   
 Thiophene

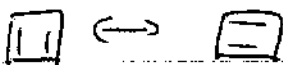
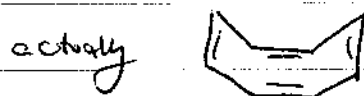
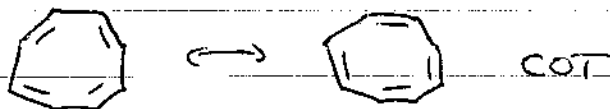
  
 $6\pi e^-$

Skip 16-4

what if  $4n+2 \neq \text{integer?}$



NOT Aromatic  
unstable!



resonance

isolated only at  $4k$

$4\pi e^-$

$$4n+2 = 8 \quad n \neq 1, 2 \dots$$

non-aromatic!

Annulenes



$$4n+2 = 10$$

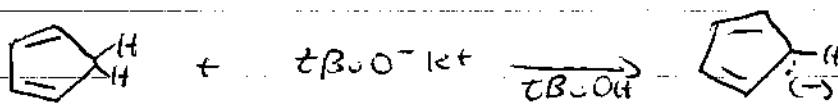
[10] Annulene

$$n = 2$$

aromatic  $\rightarrow$  is planar

Skip 16-7

## Aromaticity of Hydrocarbon Anions & Cations



cyclopentadiene

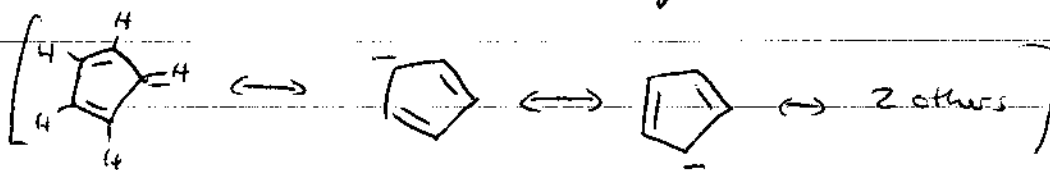
Strong acid (relative to  $\text{CH}_4$ )

$\text{pK}_a \sim 15$

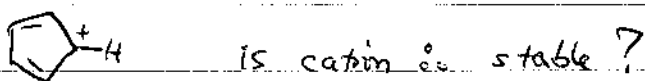
cyclopentadienyl anion

$4n + 2 = 6 \quad n = 1$

How can it lose an  $\text{H}^+$  that easily? Aromatic



But, can also draw this many resonance structure for cation:

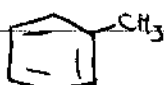


NO, 4n e- NOT just resonance structures then!

Read 16-8 to 16-9

## Nomenclature of Aromatics

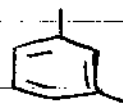
Benzene



toluene  
methyl benzene



1,2-dimethyl benzene  
o-xylene



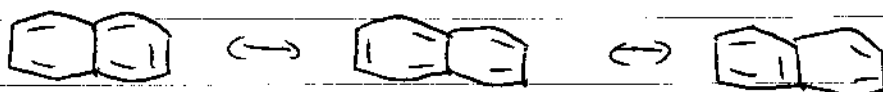
1,3-dimethyl benzene  
m-xylene



naphthalene

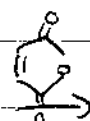
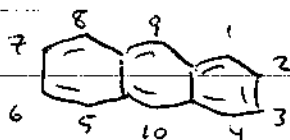


biphenyl

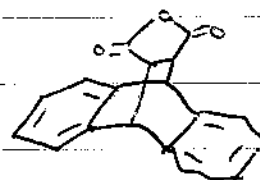


all resonance structures are NOT equal

electrophiles can react at certain positions  
more than others

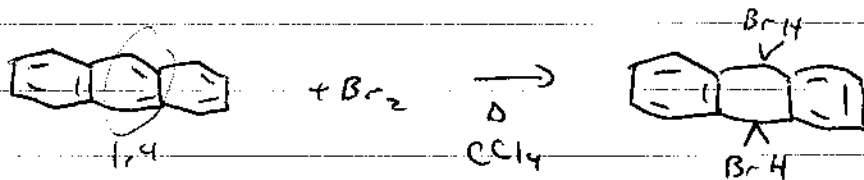
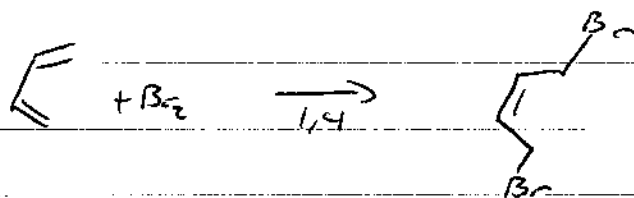
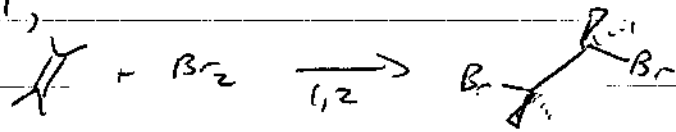


MA  
2h  
100°C

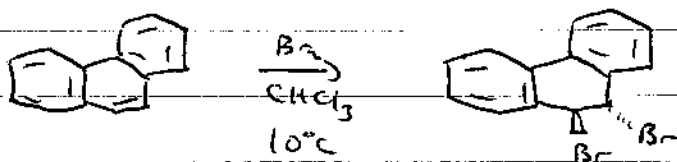


highest e<sup>-</sup> density at 9,10 positions

Recall,



Same w/ phenanthrene



Skip 16-13