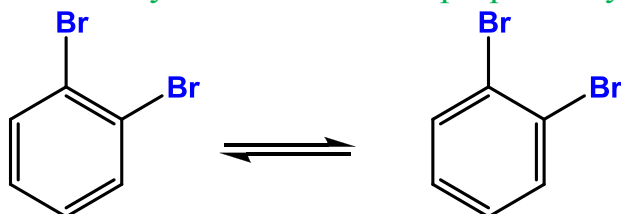


Overheads: - Outline

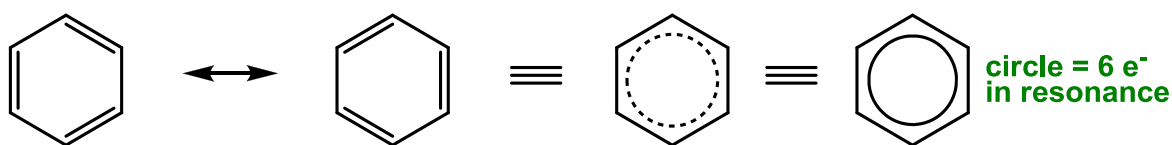
Recap Chem 241: Benzene & Resonance

1860's: cyclic structure first proposed by Kekulé

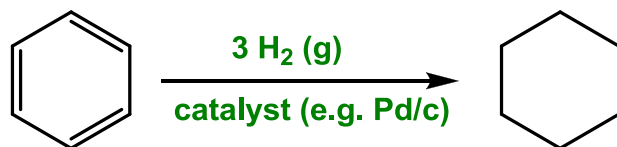


equilibrium used to explain why these two structures are the same

Now know: actually resonance hybrid:

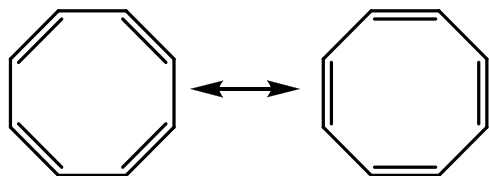


Resonance = Stability:



-120 per C=C

ΔH° (expected)	= -360 kJ/mol
ΔH° (actual)	= -208 kJ/mol
<hr/>	
"resonance energy" = 152 kJ/mol	



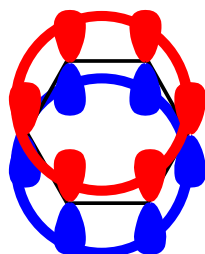
all because of resonance?

has just as much resonance as benzene
NO unusual stability!!
 resonance is **ONLY** part of the story



Benzene is Aromatic: \Rightarrow special kind of cyclic compound with unusual stability
 \Rightarrow named because of "aroma" of benzene

In order to be Aromatic, 2 criteria must BOTH apply:

- 1) Must have an uninterrupted ring of atoms with a p orbital on each atom in the ring
 \Rightarrow gives a cloud of electrons above and below ring





- like a donut with chocolate on both sides!
- In order for this to occur, the molecule must be:
 - a) cyclic
 - b) planar (flat) so that all orbitals overlap
 - c) have a p orbital on each atom



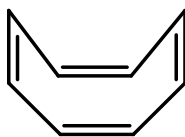
Huckel's Rule: to be aromatic, a compound must have $4n+2$ π electrons (where n = any integer: 0, 1, 2, etc.)

Antiaromatic: a compound that fits rule #1, but NOT rule #2
 ↳ cyclic, flat ↳ NOT $4n+2$
 p orbital on each atom

⇒ worse than if no resonance at all!



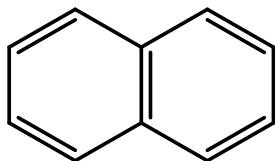
bends



not flat, so neither rule #1 nor rule #2 fit
 \therefore neither aromatic nor antiaromatic

**** If molecule can bend to avoid being antiaromatic it will**

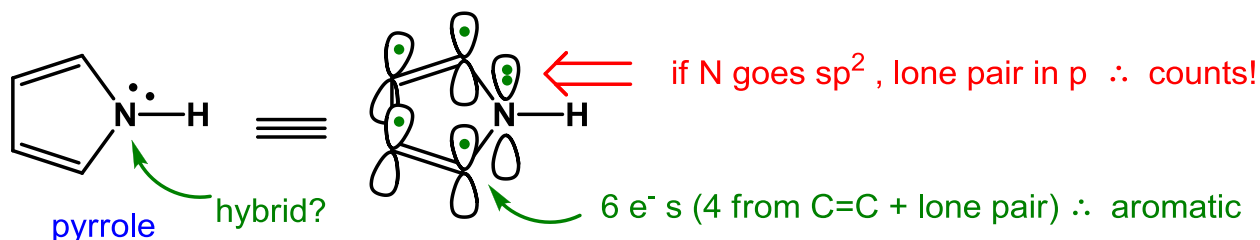
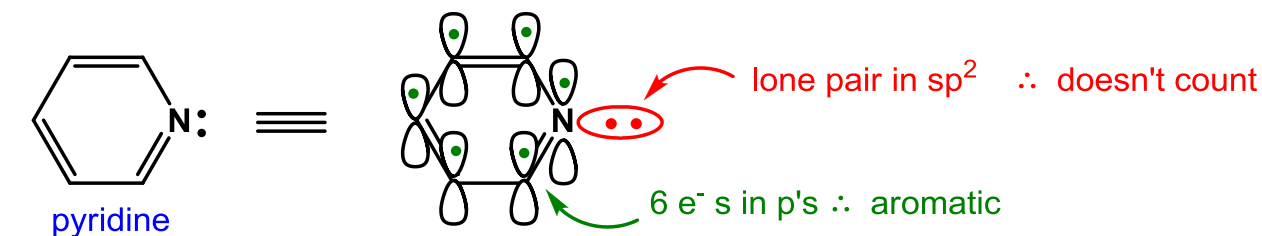
1) 2 or more joined (fused) rings:



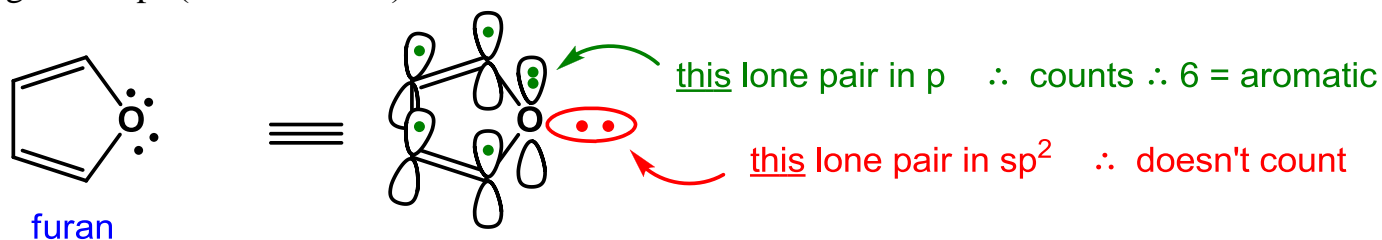
naphthalene (mothballs)
5 pairs = aromatic

2) Atoms other than C in ring:

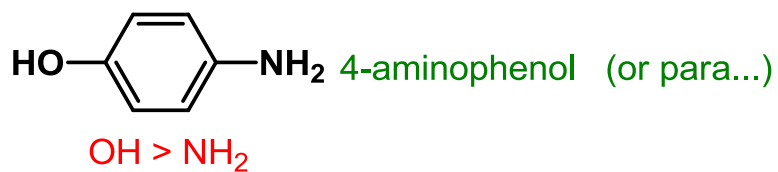
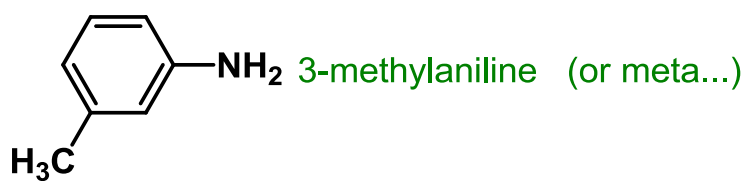
- lone pairs on O, N etc count only if in p orbitals (part of "resonance")



⇒ heteroatom can go sp^2 and put lone pair in p **if doing so will make it aromatic**
⇒ if heteroatom is already part of a double bond, p is already "used" so lone pair goes in sp^2 (doesn't count)



Examples:



Other Terminology:

