MTW

Thurs. 4/27/17

Aromaticity

Hückels Rule

1. Monocylic → one ring
2. Planar/Flat
3. All atoms have a 2p orbital in ring
   ↳ all atoms are sp^2 hybridized
4. $4n+2$ rule where n = some # (whole number, Integer) $(0, 1, 2, \ldots)$
   ↳ 6 π e^-, 2, 10, 14, 18 π e^-s

Aromatic  6 π e^- = 3 x double bonds = 3 x 2 π e^- = 6

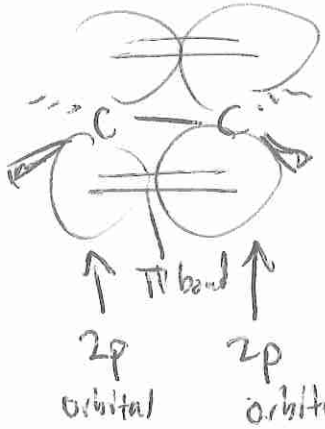
Recall a double bond is 2 π e^-s (π e^-)

Carbocations
↓
3 bonds → 3 sp^2 hybridized orbitals → form bonds
1 C-H σ
2 C-C σ bonds

sp^2 hybridized
↓
empty 2p orbital

π e^-s in this molecule
↳ 1 C=C → 2 π e^-
↳ 1 carbocation → 0 π e^-s
↳ 2p (empty) orbital

Double Bonds = Overlapping 2p orbitals

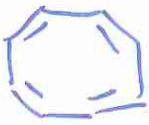


Aromatic
↓
Hückils rules are obeyed!

Anti-Aromatic → Very unstable

1. Monocyclic
2. Planar / Flat
3. All atoms have a 2p orbital
4. $4n$ π e^-s $n = 1, 2, 3$
   - ↳ 4, 8, 12, 16

$4\ \pi e^-$



If forced flat
↓
would be anti-aromatic

Drawn in IMAX 3D

Not Aromatic

↳ b/c it's not flat

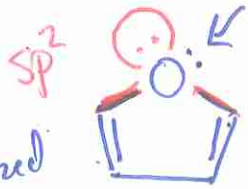
(1) What if sp^3 → 4x sp^3 hybrid. orbit.
0x 2p orbitals

L.P. → sp^3

O atom have 2p? NO

Not aromatic

(2) What if sp^2 → 3x sp^2 hybrid orbit.
1 2p orbital



Lone pair in sp^2 hybridized orbital is not in a 2p orbital

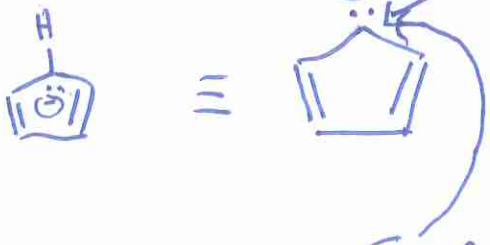
↓

Not in π-system

6 π e^- → Aromatic

To be in the π-system all e^-s have to be in a 2P orbital

If this is _____ hybridized it is _____.

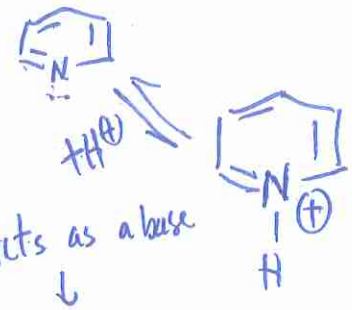


sp^3 — not aromatic

sp^2 — aromatic

In fact sp^2 hybridized → b/c aromatic

Good Base

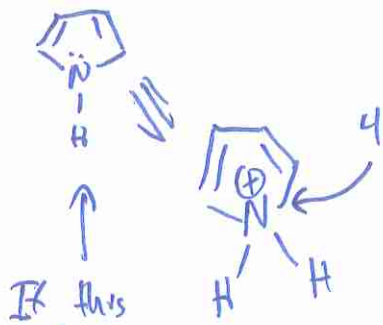


Acts as a base

↓

Doesn't lose aromaticity

Aromatic



4 bonds → sp^3

↓

Not aromatic

If this acts as a base → lose aromaticity → Not happy → so its not a good base