



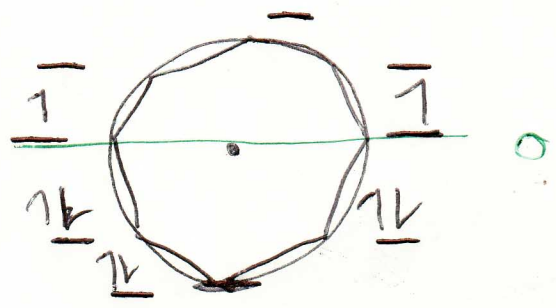
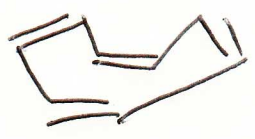
vs



- unusually stable due to cyclic conjugation
- C-C bonds are equal

- unusually unstable due to cyclic conjugation
- definite distinction between single + double bonds

Frost Circle

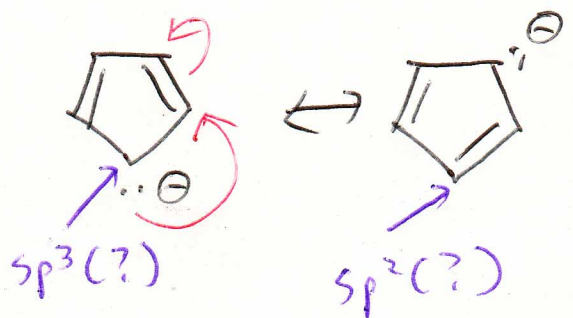


COT
cycloocta-1,3,5,7-tetraene

If COT was forced to be planar, two π -electrons that otherwise would be in bonding MOs are instead pushed into higher-energy non-bonding orbitals (not favorable). As such, the true structure of COT is distorted, so that the 4 π bonds avoid each other.



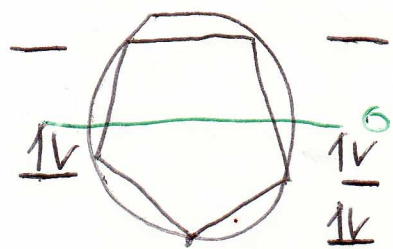
pKa ~ ~~20~~ 16



Cyclopentadiene

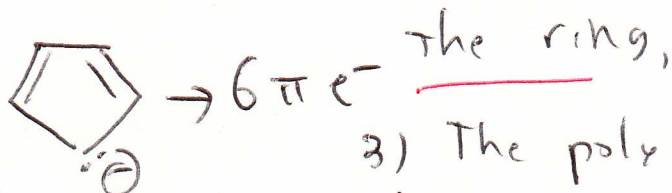
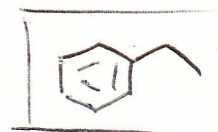
The cyclopentadienyl anion is completely delocalized. Although its structure appears to contain a carbon that is sp^3 hybridized, this is only because it is a resonance structure that fails to properly show the true structure of the molecule.

Frost Circle

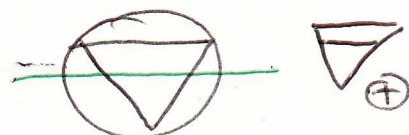


1) One vertex of a polygon is automatically positioned @ the bottom of the circle

2) # of vertices in the polygon = # of atoms in



3) The polygon is inscribed in a circle, the vertices that are at the same level as the origin represent non-bonding; below, bonding; above, anti-bonding.



Generalizations!

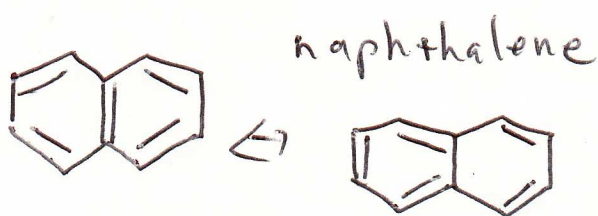
- There is always at least one bonding orbital

- Aside from the lowest-energy orbital, bonding orbitals appear in degenerate pairs.

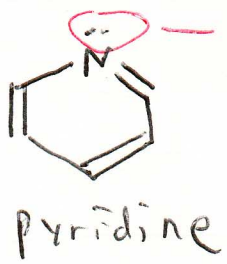
\rightarrow $4n+2$ rule - Aromatic systems will only have bonding electrons, which means the total # of $\pi e^- = 4n+2$, where $n \geq 0$

Hückel rules - A compound will be aromatic when!

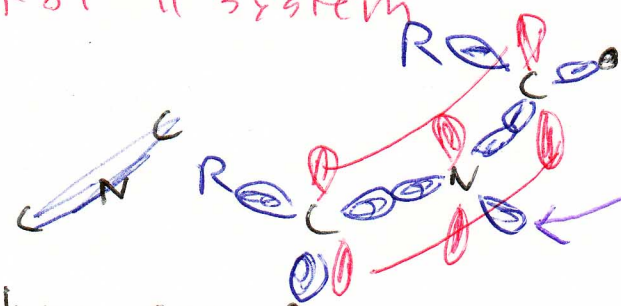
- It is cyclic;
- It is fully conjugated (in the circle)
- It is planar;
- It has $4n+2 e^-$



- ✓ cyclic
- ✓ fully conj.
- ✓ planar
- ✓ $4n+2 = 10; n=2$

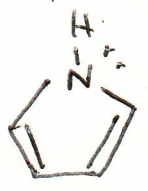


not part of π system



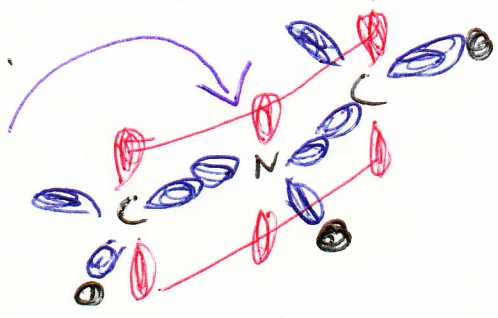
lone pair is in sp^2 orbital, which is \perp to π system

✓ aromatic, since there are only 6 πe^- in a planar, cyclic, conjugated system,

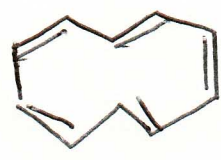
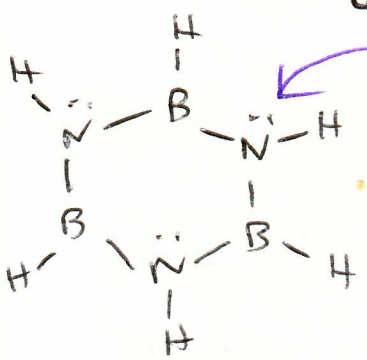


sp^2 !!!

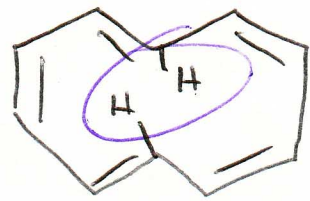
Although nitrogen appears to have sp^3 hybridization, it is energetically far more favorable for it to be sp^2 hybridized, since it would then become part of an aromatic system.



lone pair



- ✓ cyclic
- ✓ 10 πe^-
- ✗ not planar



Due to steric hindrance (the two H being pointed @ each other), the molecule is distorted and non-planar, so it is not fully conjugated.