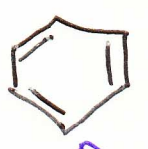


2/29/12

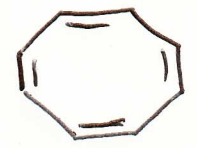


anti-aromatic - cyclization causes instability

aromatic - cyclization causes notable stability

Frost Circle -

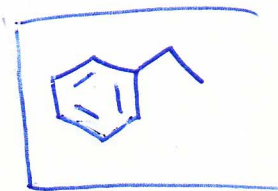
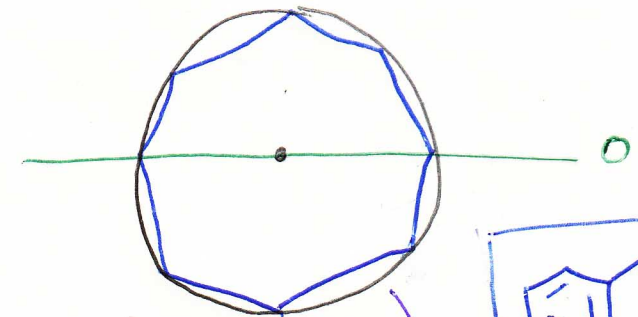
Rules for creating a Frost circle



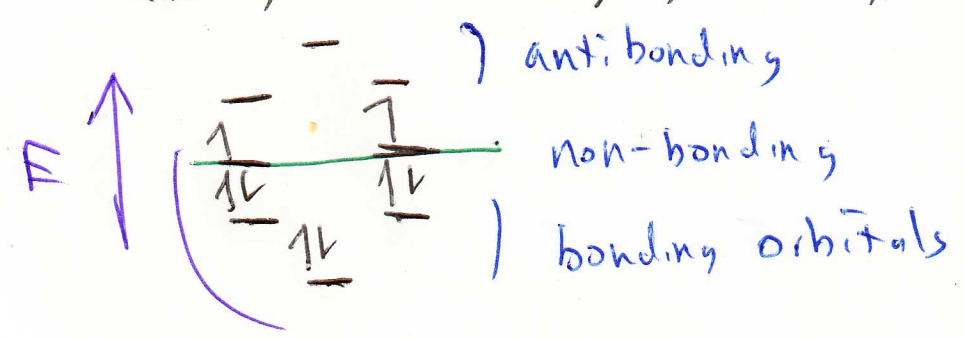
→ 8 π e⁻

COT

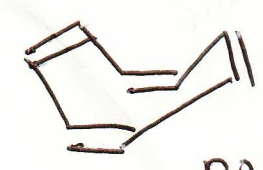
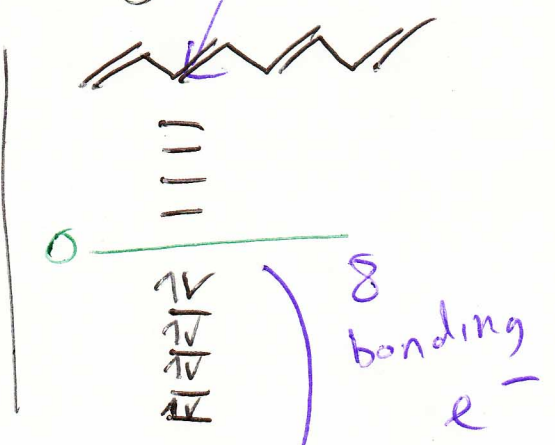
cycloocta-1,3,5,7-tetraene



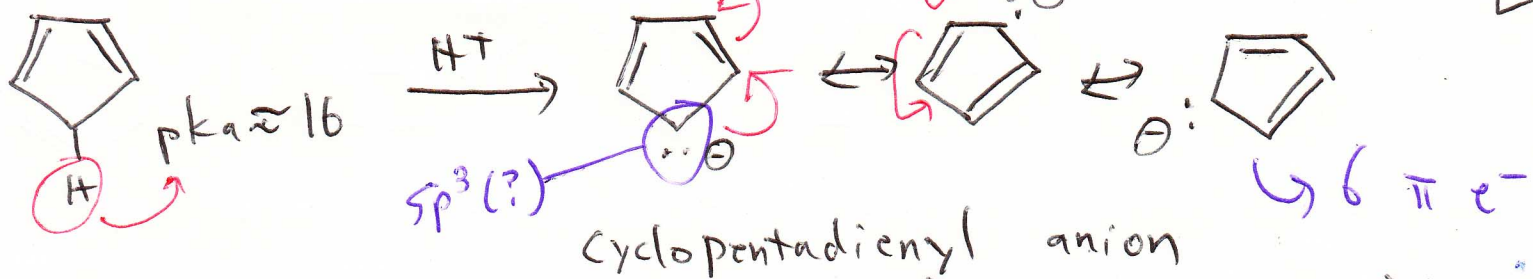
- I inscribe a polygon that has the same number of sides as the # of atoms in the cyclic system.
- One vertex of the polygon must be located at the very bottom of the circle.
- Vertices on the midline represent non-bonding MO; above, anti-bonding; below, bonding.



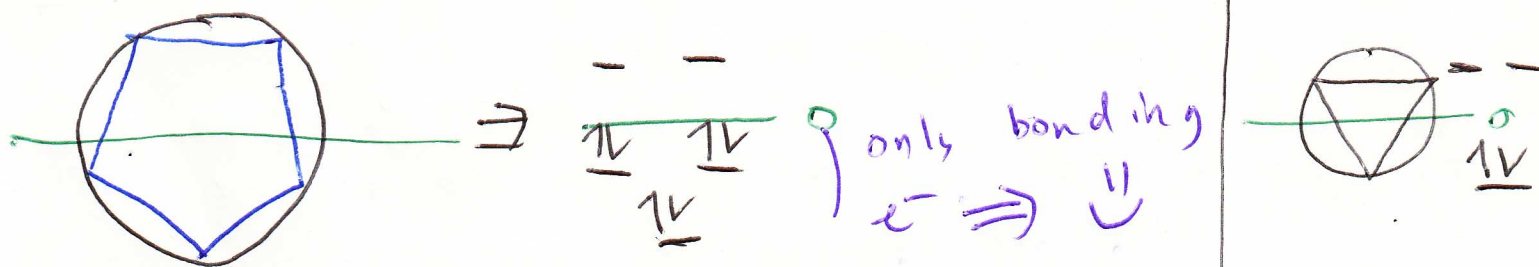
only 6 bonding e⁻



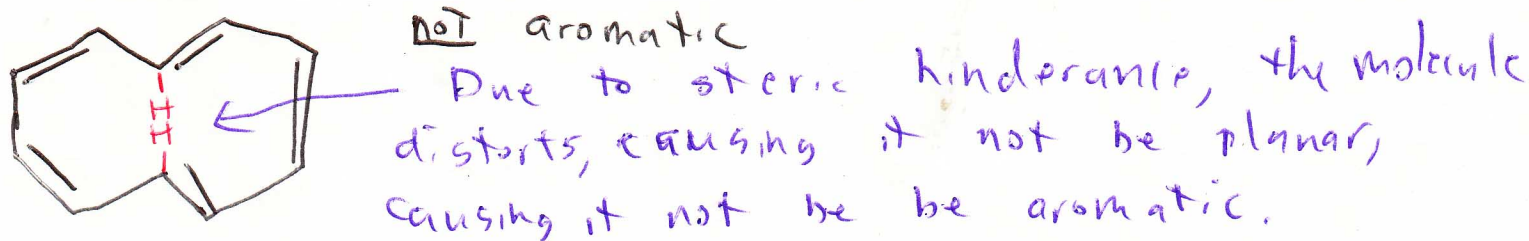
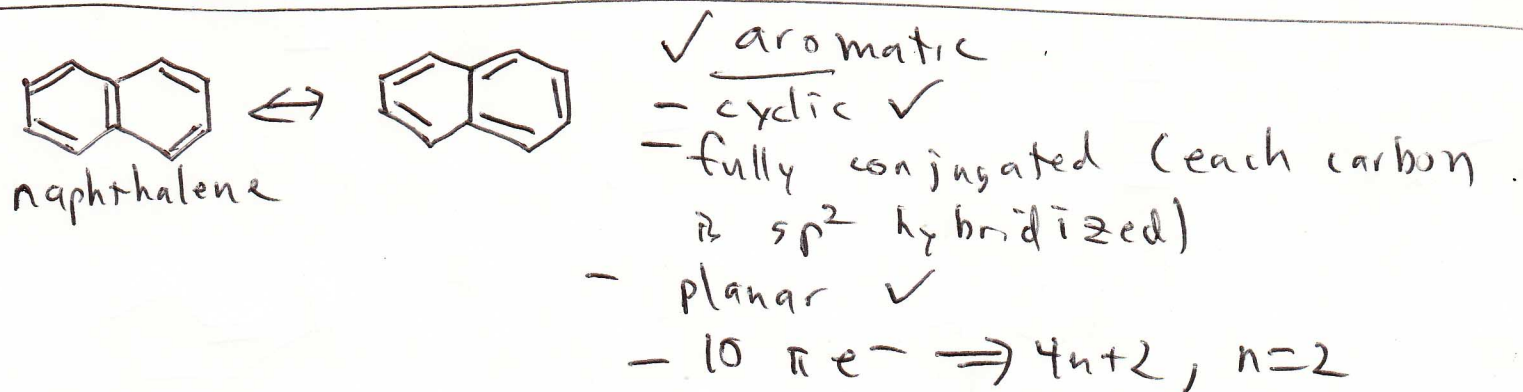
In COT, when the molecule is forced to be planar, two π e⁻ are forced into non-bonding MOs. If COT distorts, the 4 π bonds are no longer fully conjugated, so the π e⁻ would exist only in bonding orbitals instead.

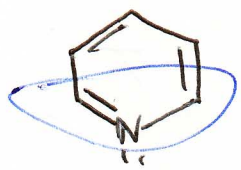


Although the cyclopentadienyl anion is written with a localized lone pair (which makes that carbon appear to be sp^3 hybridized), the written structure fails to correctly reflect the shape of CPD anion due to delocalization.



- Hückel rules for aromaticity:
- 1) cyclic
 - 2) full conjugation around the ring
 - 3) planar
 - 4) # of $\pi e^- = 4n + 2$; $n \geq 0$ (must be a whole #)

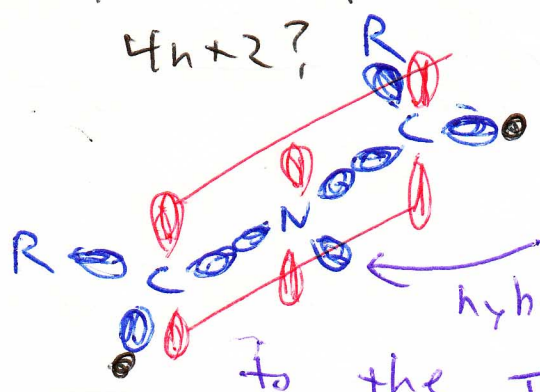




pyridine

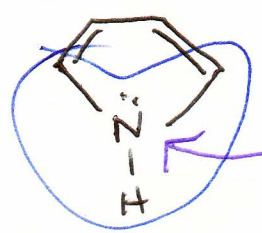
cyclic ✓ planar ✓ conjugated ✓

$4n+2?$



✓ aromatic

lone pair is in a sp^2 -hybridized orbital and is \perp to the π system; the lone pair does not delocalize.

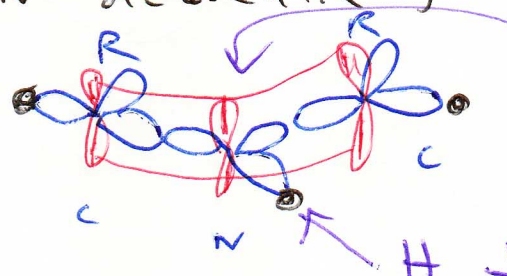


pyrrole

cyclic ✓ planar ✓ conjugated?

sp^2 !!!!

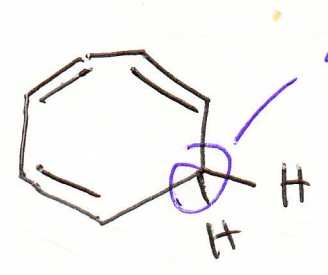
The nitrogen in pyrrole is sp^2 hybridized due to the fact that energy is released by the lone pair on N delocalizing with the neighboring π bonds.



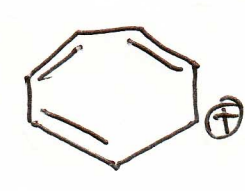
lone pair part of π system

✓ aromatic

H \perp to π system



sp^3



cycloheptatrienyl cation

\rightarrow tropylium ion