Aromaticity - Lecture 2

Note Title 2/17/2014

Announcements: 1) Discussion sections, labs & office hours begin this week!

(Schedule of discussion sections & office hours on course website.)

Lab scheduling → Ms. Linda Staib (102 BRL)

Disability Accommodations

2) Lab: Canvas website

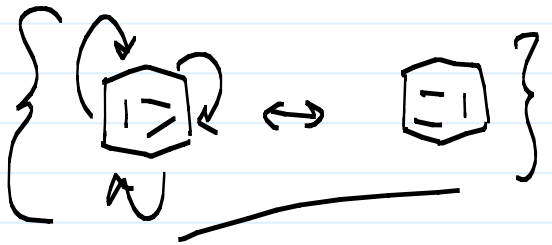
Quizzes due by midnight on day before your lab.

Pre-lab assignment

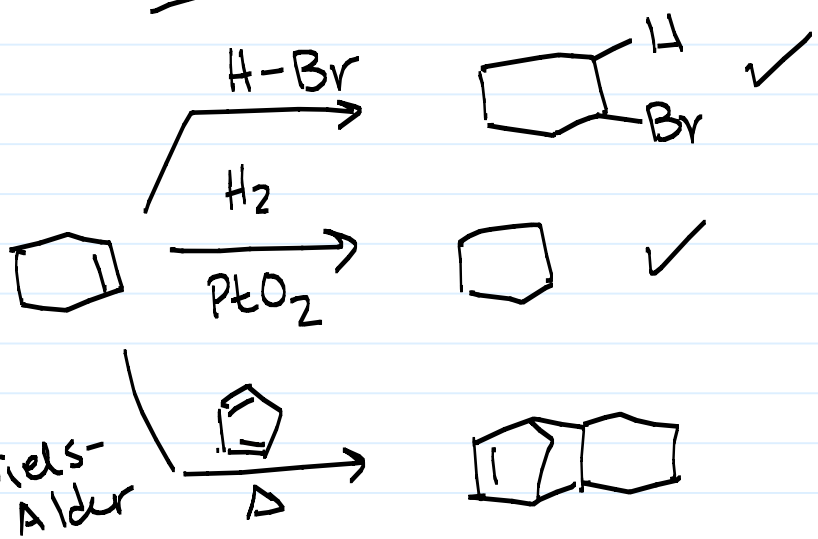
3) If you are transferring your lab grade from previous semester, please see me after class.

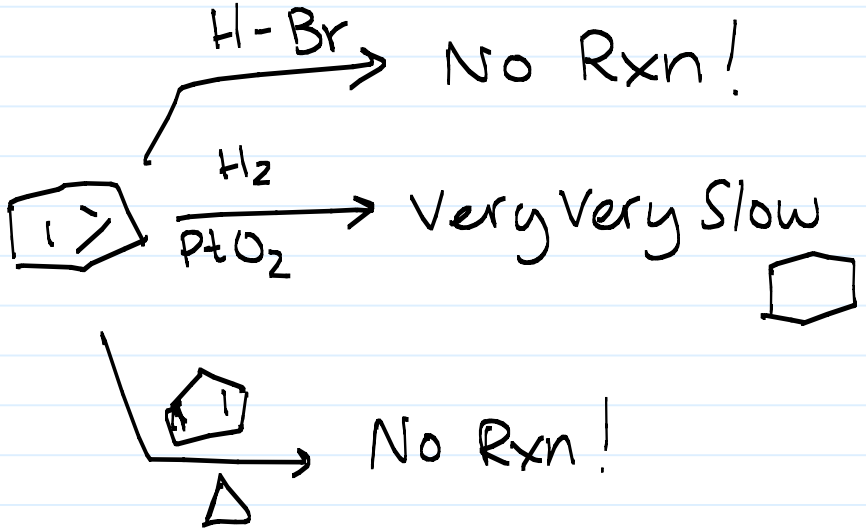
4) Added to course website: notes, practice problems

Recall: Benzene: Extra stability from delocalization of e⁻s in the π-system



How much extra stability? ~30 kcal/mol





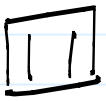
Is C_6H_6 the only aromatic compound? NO.

4 Criteria for Aromaticity: Molecule must be:

1) Cyclic
2) Fully conjugated → every atom has p orbital parallel to π-system
3) Planar (so p orbitals can overlap)
4) Hückel's Rule: $(4n+2)$ π e⁻s, n = integer (0, 1, 2, 3, ...)

ex: 

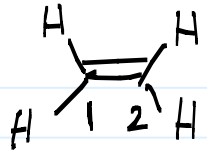
1) Cyclic ✓
2) Fully conj ✓
3) Planar ✓
4) $6\ \pi e^- \underset{n=1}{=} 4n+2$ ✓

ex: 

Not aromatic
ANTI-AROMATIC

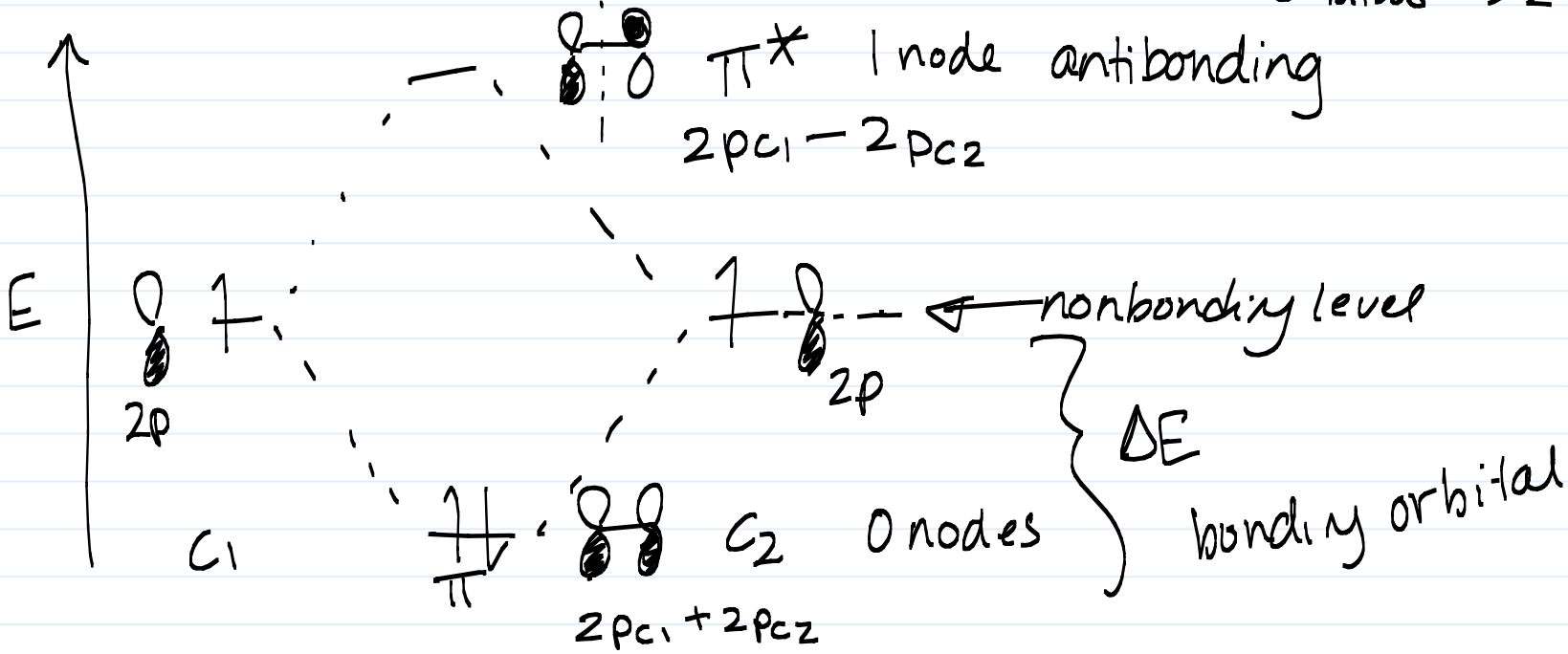
1) cyclic ✓
2) fully conj ✓
3) planar ✓
4) $4\ \pi e^- = 4n+2 \rightarrow n = 1/2$ ✗

Why is 4n+2 so important? Bigger MO picture...

Ethylene 

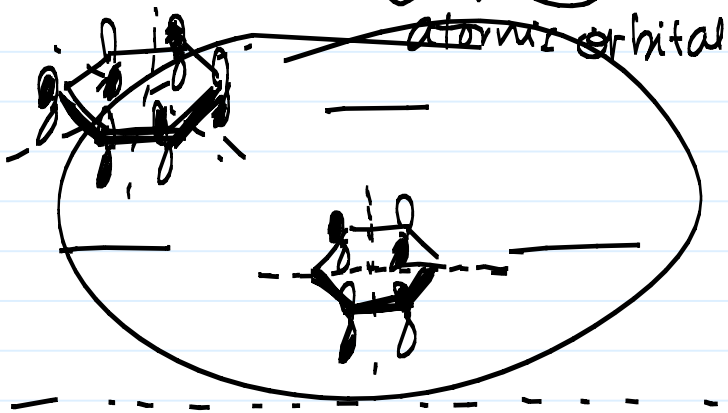
π-bond = $\underbrace{2p_{c_1} + 2p_{c_2}}$

2 atomic orbitals → 2 molecular orbitals



Benzene:  6 2p orbitals → one on each C.

atomic orbitals → 6 molecular orbitals

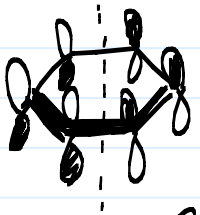


3 nodes

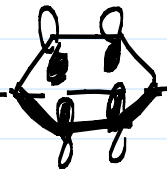
2 nodes } antibonding

E

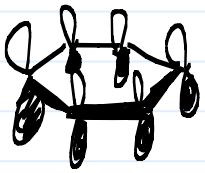
nonbonding level (p-orbital)



1 node



} bonding

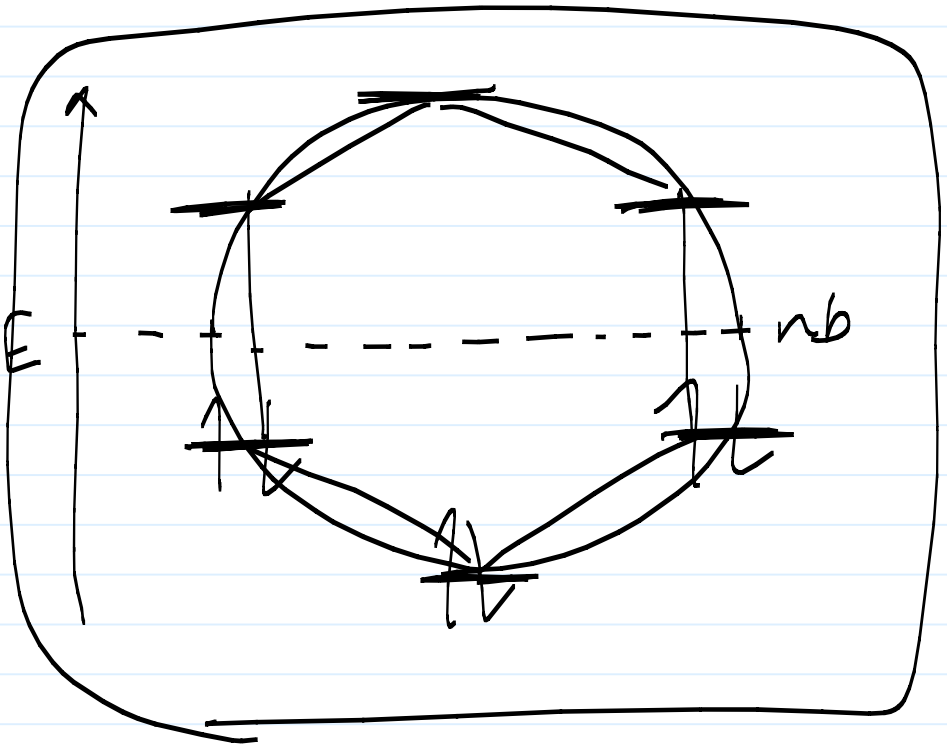


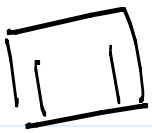
0 nodes

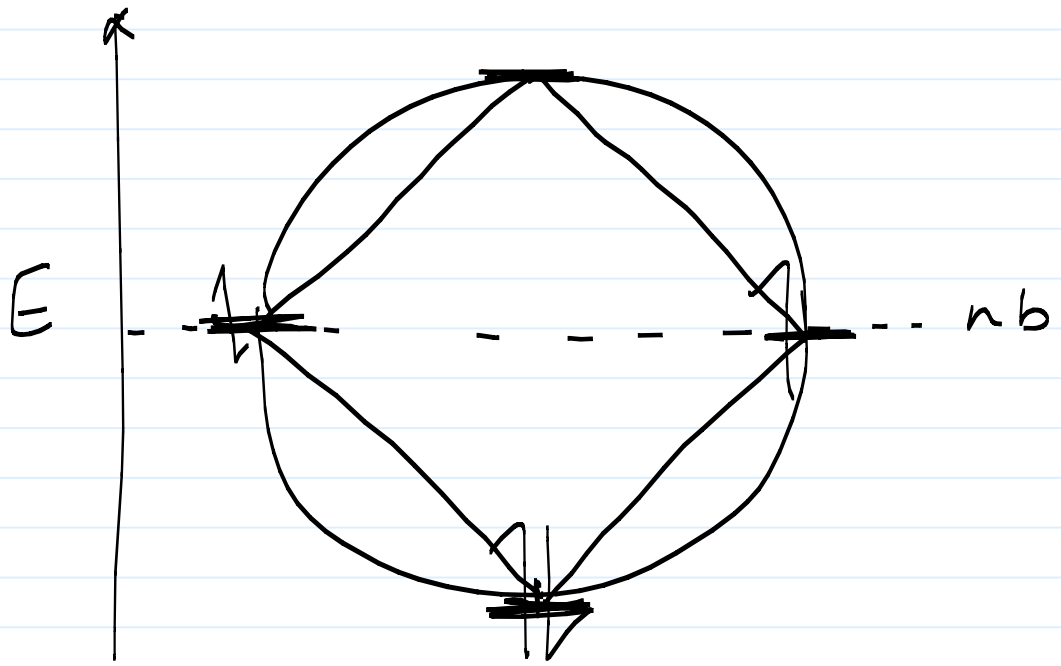
Frost Magic Circle → Easy → generates MO diagram for π system for aromatic compounds.

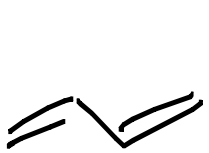
Protocol:

1) Draw circle (centered on nonbonding level)
2) Draw ring of molecule w/ vertex/point down.
3) Where ring needs circle → MO (π)
4) Fill in e-s (bottom up)



ex:  $4n+2=4$, $n=1/2$ X Anti-aromatic

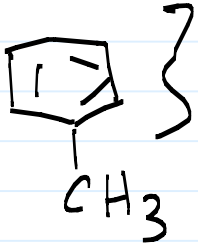




1) cyclic ✗

1) cyclic ✓

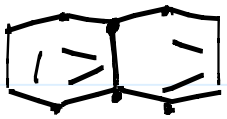
2) fully conj ✗



toluene

Substituted benzene → only consider aromatic piece

1) cyclic
2) fully conj
3) planar
4) $4n+2=6$, $n=1$ ✓

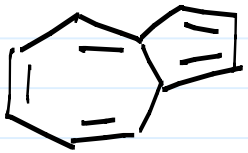


naphthalene

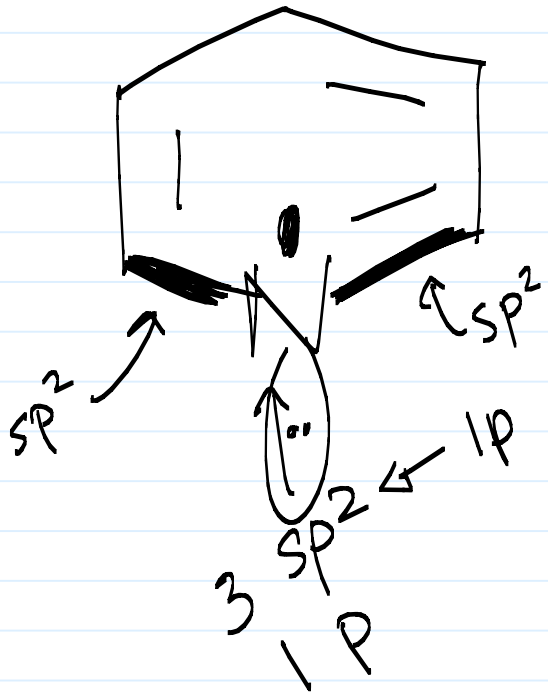
1) cyclic ✓
2) fully conj ✓
3) planar ✓
4) $4n+2 = 10, n = 2$ ✓

aromatic

Polynuclear aromatic = multiple aromatic rings



1) cyclic ✓
2) conj ✓
3) planar ✓
4) $4n+2 = 10, n = 2$ ✓

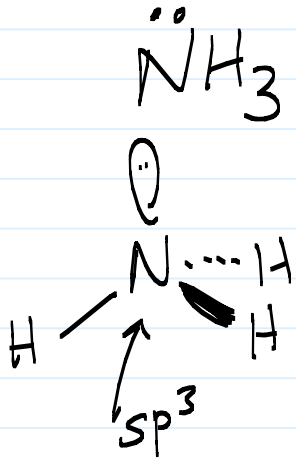


1) cyclic ✓ "heteroaromatic"

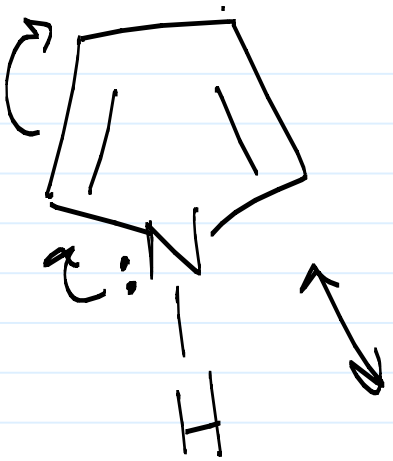
2) conj ✓

3) planar ✓

4) $4n+2=6$, $n=1$ ✓

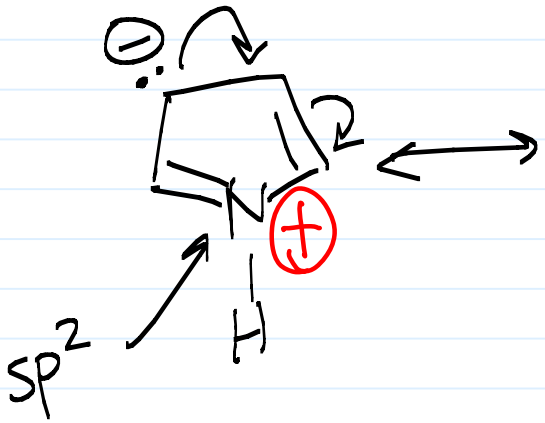


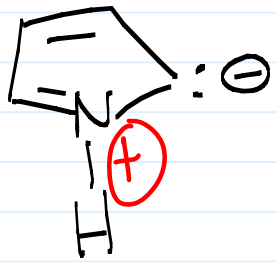
↑ lp on N ⊥ to π system ↓ doesn't count!!



pyrrole

1) cyclic ✓
2) Fully conj ✓
3) planar ✓
4) $6 = 4n+2$, $n=1$ ✓





[Please note: I forgot to put ⊕ on N in lecture. Sorry!]