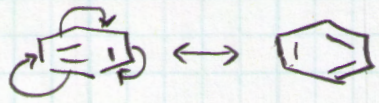
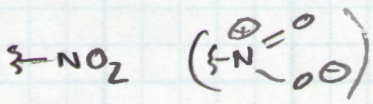
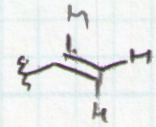
Benzene  Aromatic, molecule

what will be learned
- Naming (briefly)
- what does it mean to be aromatic
- Define/Recognize Aromatic, Non-Aromatic, Antiaromatic

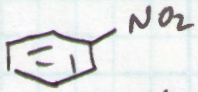


Nitro



ethenyl

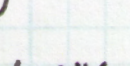
isopropyl



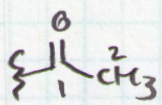
nitrobenzene

Higher priority functional groups

-ol



-amine

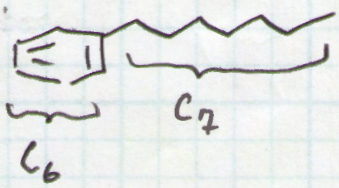


- ethanone (ketone)

benzenol (phenol)

benzenamine (aniline)

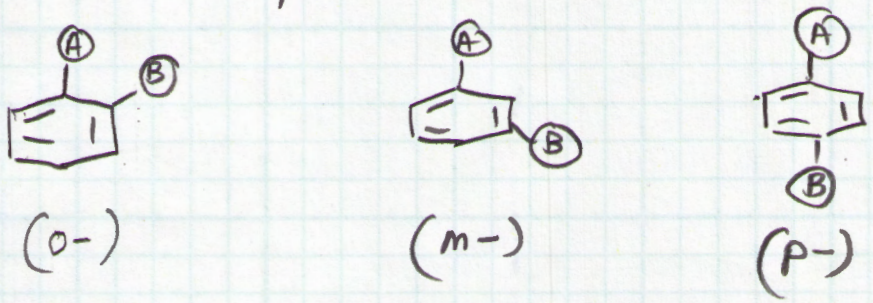
1-phenylethanone (acetophenone)



"benzene" has priority over substituents of only length.

ortho, meta, para

o- m- p-

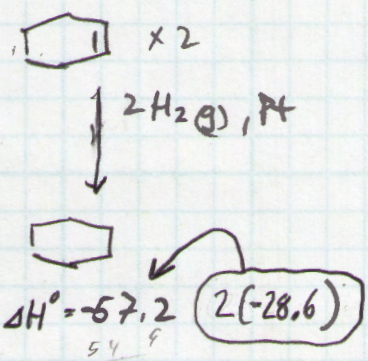


relationship betw A & B

(o-) (m-) (p-)

Resonance stabilizat^n of benzene

Earlier, we saw res stabilizat^n of conj π bonds over isolated π bonds



kcal mol^{-1}

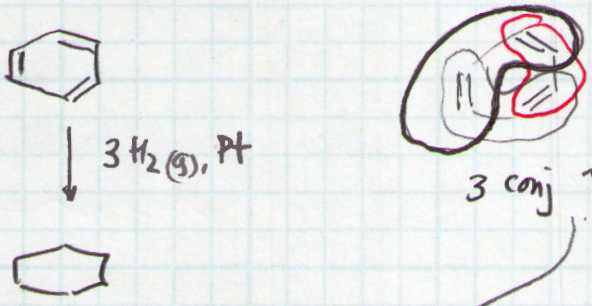
ΔH° = -57.2 (2(-28.6))

54 6

2.3

-54.9 less E release

∴ more stable by ~2.3 kcal mol^{-1} DUE TO RESONANCE of π bonds



3 conj π schemes

Predicted E release

3(-28.6) + 3(2.3) = -78.9 kcal mol^{-1}

Resonance stabilizat^n of conj π bonds

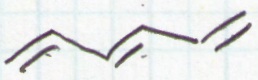
Observed!

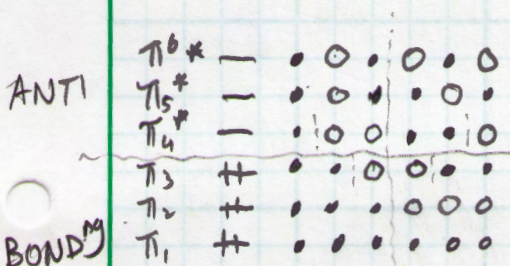
-49.3 kcal mol^{-1}

∴ benzene is more stable than a conj cyclic diene and a hypothetic cyclic triene at -78.9 kcal mol-1

The $\Delta\Delta H^\circ$ $\quad -78.9$
$\quad -(-49.3)$
$\quad -29.6$ kcal mol^{-1} → is the resonance stabilizat^n of benzene

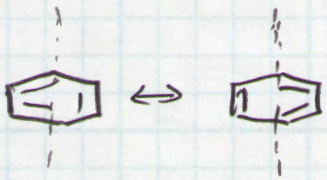
MOs of Benzene

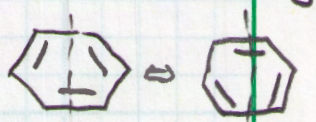
Let's Review  1,3,5-heptatriene MOs



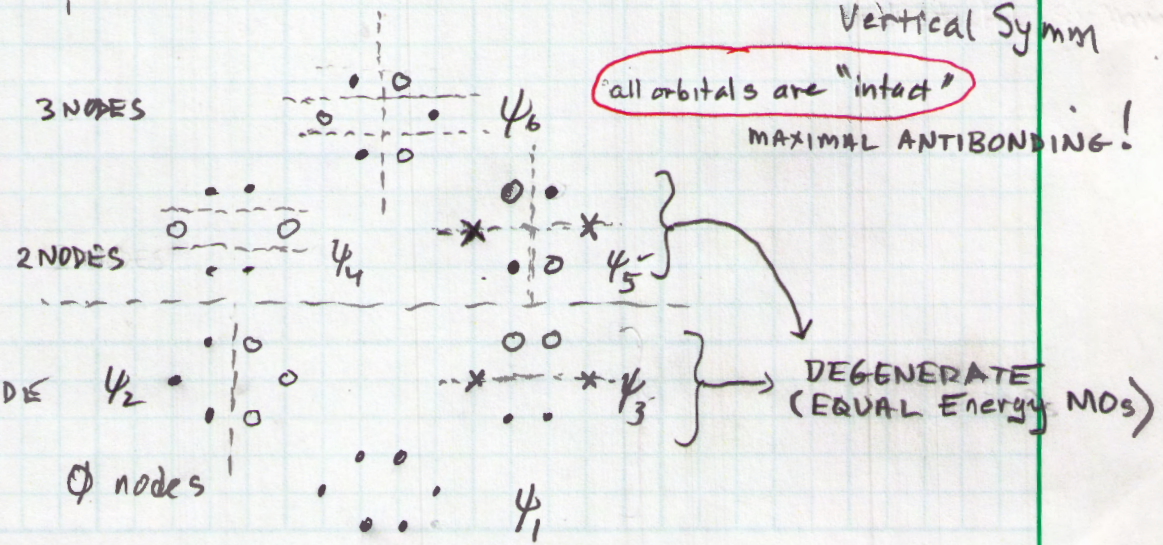
(6) EVEN # of p-orbitals make 6 MOs
NO 'x' nodes

BENZENE MOs configuration of MOs is confined by constrain cyclic geometry and symmetry (vertically)



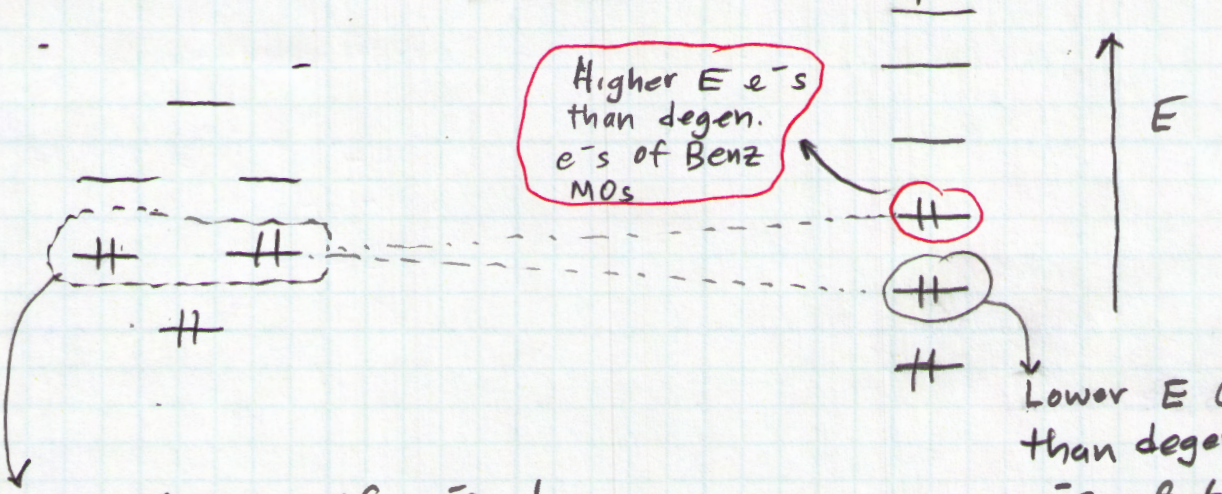
NO VERTICAL SYMM. BUT  Vertical Symm

6 p orbitals yield 6 MOs for benzene



BENZENE MOs

1,3,5 - heptatriene MOs



Lower E e⁻s than degenerate e⁻s of benzene MOs

These 2 pair of e⁻s being in lower E MOs make benzene more stable than conj. heptatriene