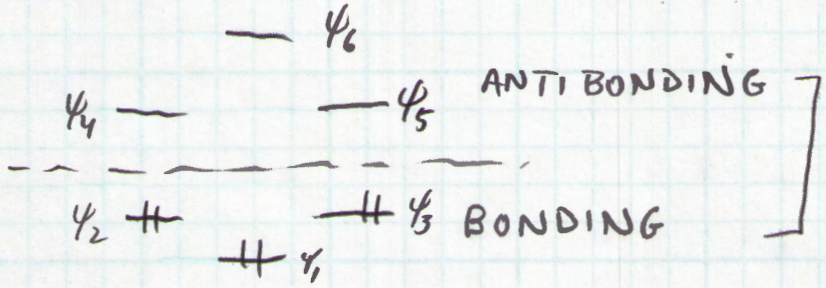
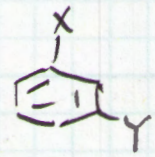
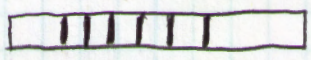
Recall the MOs of an Aromatic cmpd we looked at earlier



Large E gap i.e. needs high E photons to excite e⁻ from bonding MO to antibonding MOs

UV Absorbance

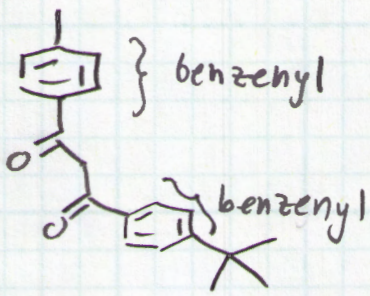




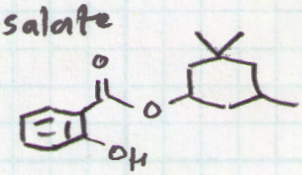
uv wavelength aborbed by the aromatic (benzene) Sample.

Sunscreens

Avobenzone

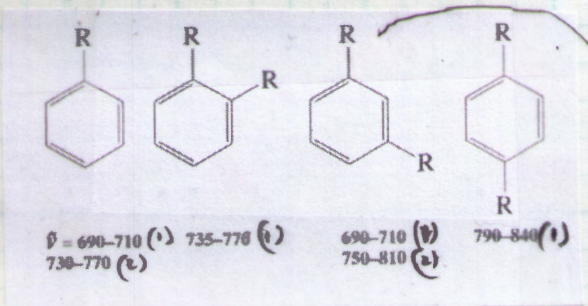


Homosalate

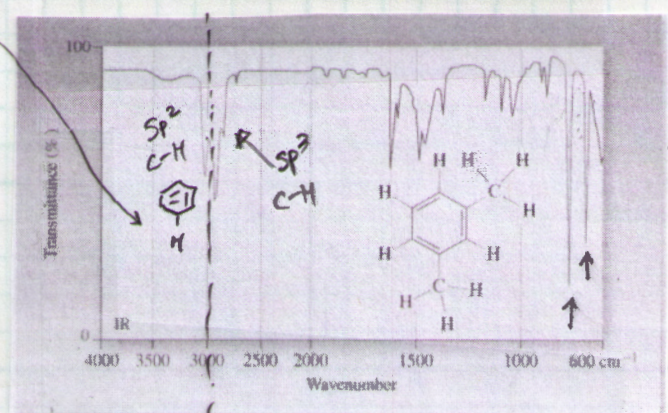


Absorb UV-light

IR



IR peaks 2+ 1 2 1



NMR

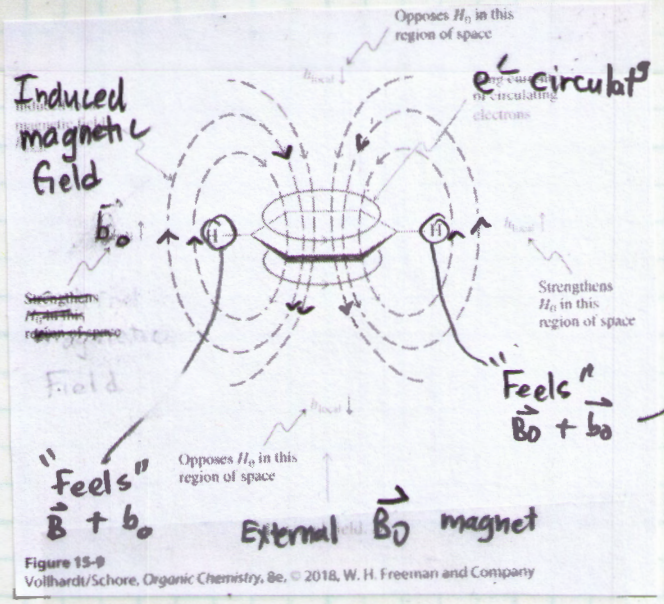
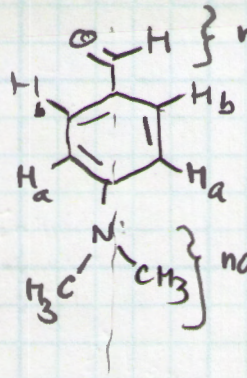
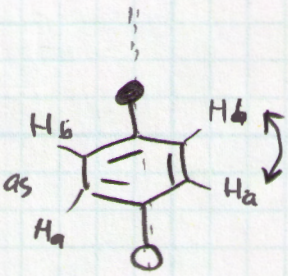


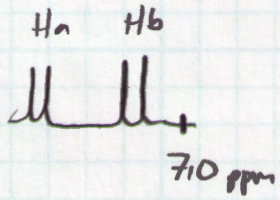
Figure 15-9
Vollhardt/Schore, *Organic Chemistry*, 8e, © 2018, W. H. Freeman and Company

→ Deshields aromatic C-H protons, appear > 7.0 ppm



symmetry can be viewed as

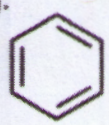




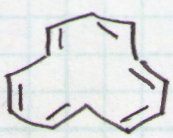
Hückel's Rule of Aromaticity.

Think of conjugated double bond systems as circuits where e^- flow is possible because the e^-s are connected by p-orbitals.

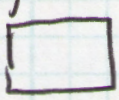
cyclic conjugated systems can only be AROMATIC if they contain $4n+2$ π e^-s where $n = 0, 1, 2, 3 \ldots$

Aromatic	Anti-Aromatic	Non-Aromatic
unusually stable	*unusually unstable*	***everything else***
•Cyclic ✓	•Cyclic ✓	Cyclic ? ✓
•Conjugated ✓ Cyclically	•Conjugated ✓ Cyclically	*Fails any one of the 4 criteria on the left* Conj. NO
•(4n+2) Pi electrons ✓	•(4n) Pi electrons ✓	4n π e⁻ ✓
•Flat ✓	•Flat ✓	Flat? NO!
e.g. 	e.g.	e.g.
benzene	**cyclobutadiene**	**cyclooctatetraene**
(resonance energy of 36 kcal/mol)	(only stable below −100 °C)	(adopts a tub-like shape to "escape" anti-aromaticity)

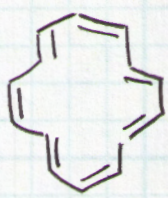
List the following as Aromatic (A), Anti-Aromatic (AA) or Non-Aromatic (AN) given the following observations.



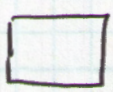
nearly planar



A, AA or AN?



planar



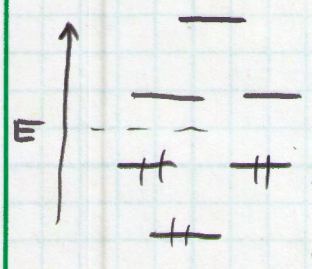
A, AA or AN?

Pattern of MO of cyclic conj π systems determined by Hückel (1931)

> x+1 = conj π bonds in cyclic system w/o intervening saturated carbon

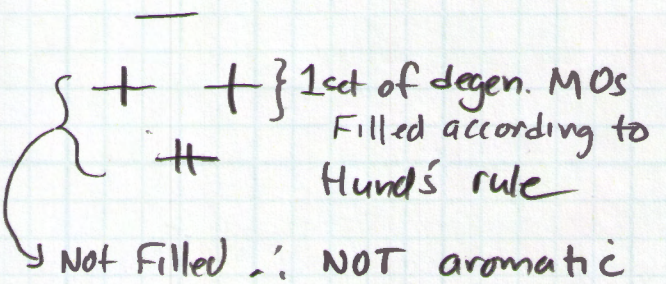
x+1 = 3 conj π bonds in cyclic system

x = 2



x + 1 = 2

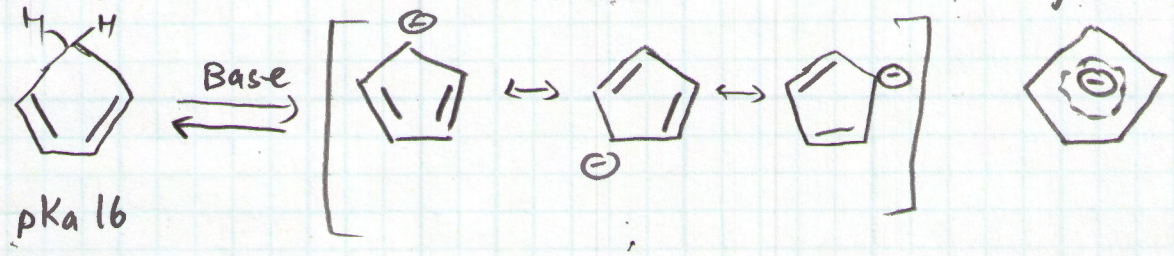
x = 1



if obs shows this molecule is nearly planar, then anti-aromatic

if obs. show not planar, then non-aromatic

Charged Aromatics

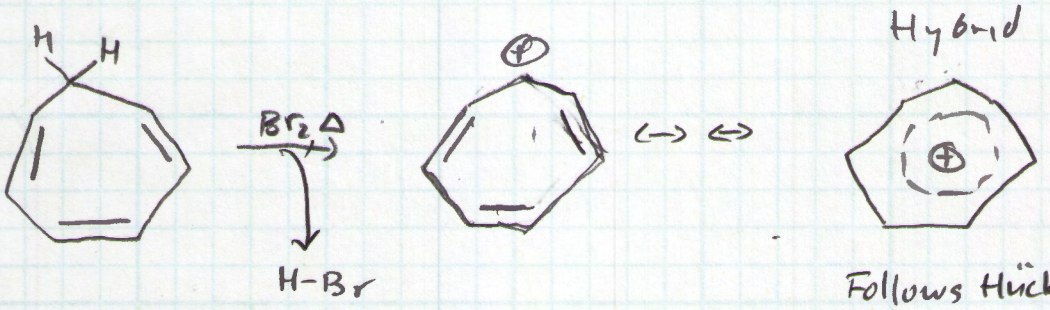


pKa 16

6 e⁻, 6 p orbitals, conj π system

$4n+2 = 6$, $n = 1$ Follows Hückel ∴ Aromatic

- Cyclic ✓
- conj cyclically ✓
- $4n+2$ π e⁻ ✓
- Flat ✓



Follows Hückel

- Cyclic ✓
- conj cyclic ✓
- $4n+2$ e⁻ ✓
- Flat ✓ ∴ Aromatic