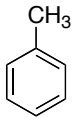
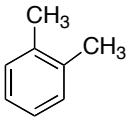
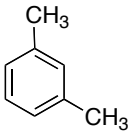
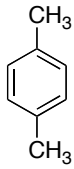
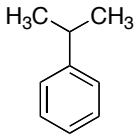
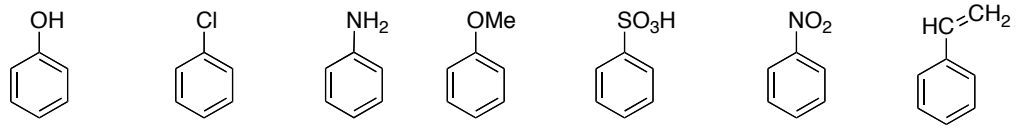
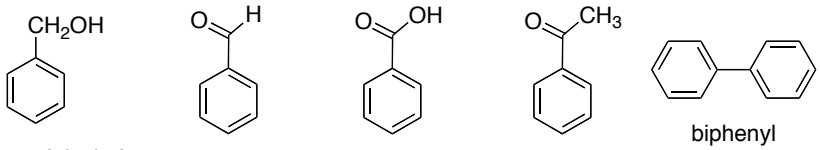
Aromatic Compounds

						
Common Name	benzene	toluene	*ortho*-xylene	*meta*-xylene	*para*-xylene	cumene
IUPAC		methyl-benzene	1,2-dimethyl-benzene	1,3-dimethyl-benzene	1,4-dimethyl-benzene	isopropyl-benzene

Other aromatic compounds:



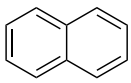
phenol | chlorobenzene | aniline | anisole | benzene sulfonic acid | nitrobenzene | styrene



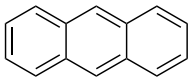
benzylalcohol or phenylmethanol | benzaldehyde | benzoic acid | acetophenone | biphenyl

More Aromatic Compounds

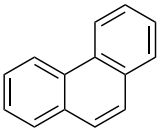
Polycyclic Aromatic Compounds



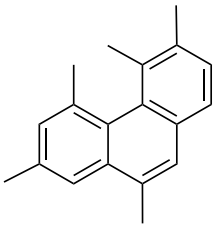
naphthalene



anthracene



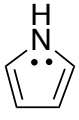
phenanthrene



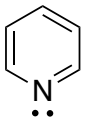
2,4,5,6,10-pentamethylphenanthrene

Heterocyclic Aromatic Compounds

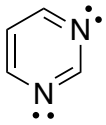
furan



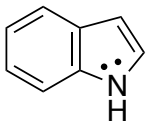
pyrrole



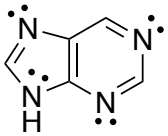
pyridine



pyrimidine



indole



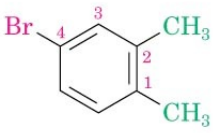
purine

Naming Aromatic Compounds (Benzene as a Substituent)

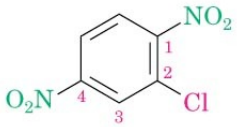
- If the the alkyl chain is larger than the ring use it as the parent
- When a benzene ring is a substituent, the term **phenyl** is used (for $C_6H_5^-$)
  - You may also see "Ph" or "ϕ" or "C_6H_5"
- Remember that **benzyl** refers to "$C_6H_5CH_2^-$"

Naming Aromatic Compounds (Benzenes with More Substituents)

- Choose numbers for the lowest possible values
- List groups alphabetically (hyphenated between) numbers
- Common names, such as toluene can serve as root name (as in TNT)



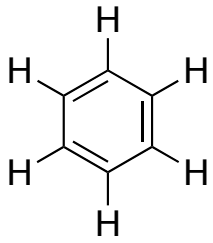
4-Bromo-1,2-dimethylbenzene

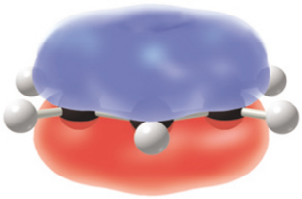


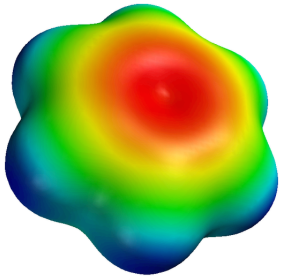
2-Chloro-1,4-dinitrobenzene

2,4,6-Trinitrotoluene (TNT)

Structure of Benzene

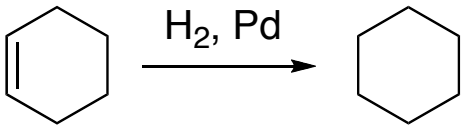


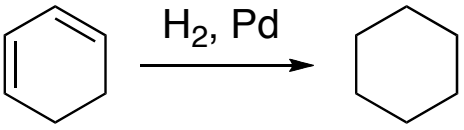


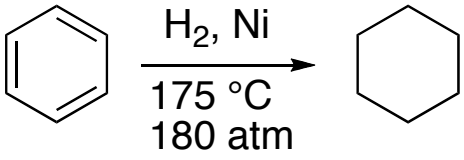


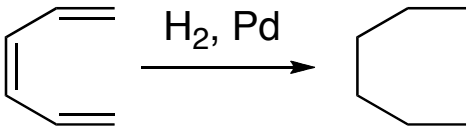
- All its C-C bonds are the same length (1.39 Å)
  - between length of normal single and double bonds
- Electron density in all six C-C bonds is identical
- Structure is planar

Stability of Benzene (Heats of Hydrogenation)





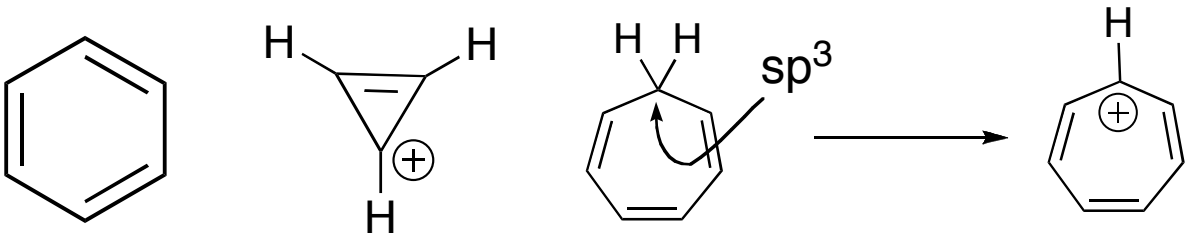




Aromaticity and the 4*n* + 2 Rule

1. monocyclic cmp (i.e. don't look at anthracene, etc)
2. All atoms in the ring must have a p-orbital (sp^2 atoms)
3. The p-orbitals must overlap...the cmp must be flat and the overlap unbroken
4. π-cloud must contain 4n+2 electrons (Hückel's Rule)

   n = 0,1,2,3,4,5....
   Therefore, compounds with 2,6,10,14,18 electrons will be aromatic
   ALL the rules must be followed to be aromatic!
   Huge energy advantage to being aromatic!

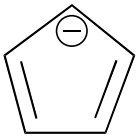


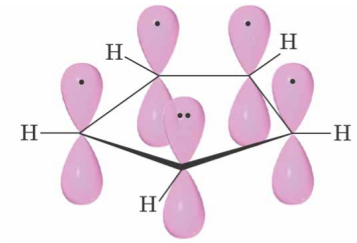
Antiaromatic Compounds

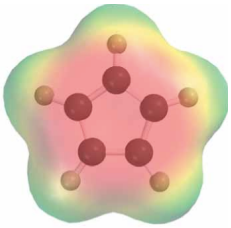
1. monocyclic cmp (i.e. don't look at anthracene, etc)
2. All atoms in the ring must have a p-orbital (sp^2 atoms)
3. The p-orbitals must overlap...the cmp must be flat and the overlap unbroken
4. π-cloud must contain 4n electrons

n = 0,1,2,3,4,5....
Therefore, compounds with 4,8,12,16,20 electrons will be antiaromatic
ALL the rules must be followed to be antiaromatic!
Basically, nature avoids...use to explain why stuff doesn't happen

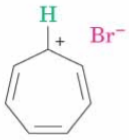
Aromatic Ions



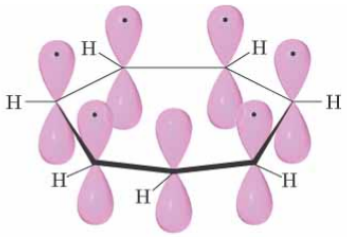


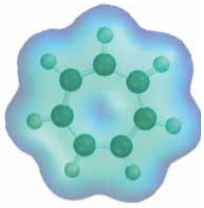


Aromatic cyclopentadienyl anion with six π electrons



Cyclohepta-trienylium bromide

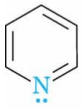


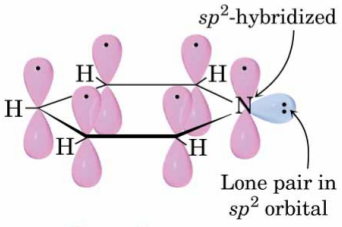


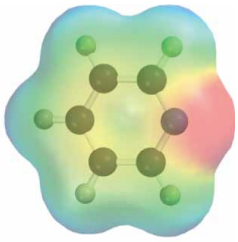
Cycloheptatrienyl cation
six π electrons

Aromatic Heterocycles

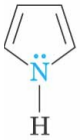
- A **Heterocycle** is a cyclic compound that contains an atom or atoms other than carbon

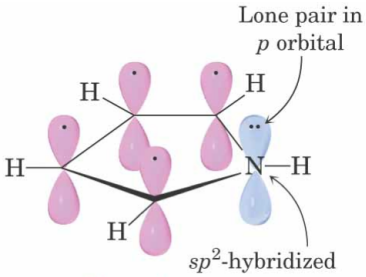


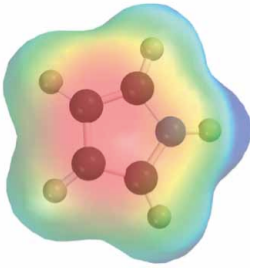




Six π electrons

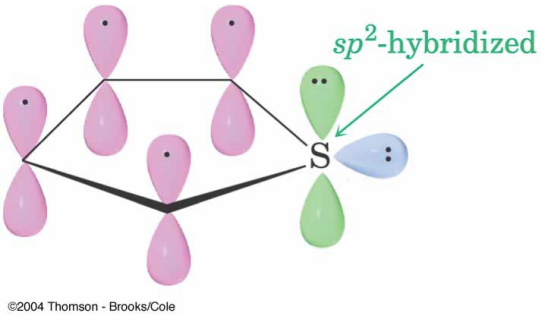






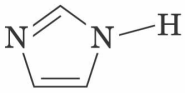
Six π electrons

More Aromatic Heterocycles

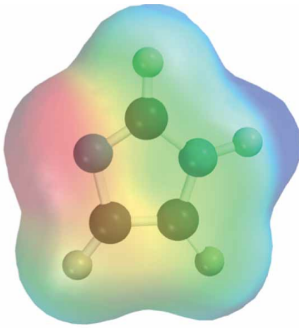


Thiophene

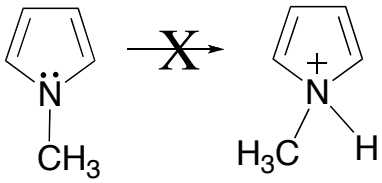
Furan

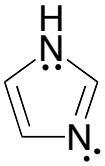


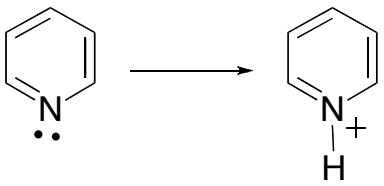
Imidazole

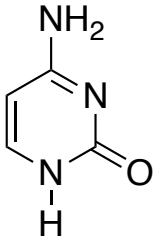


Special Cases Pay Attention!

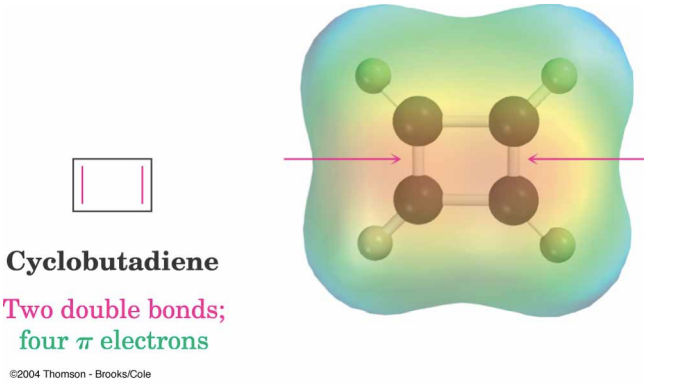




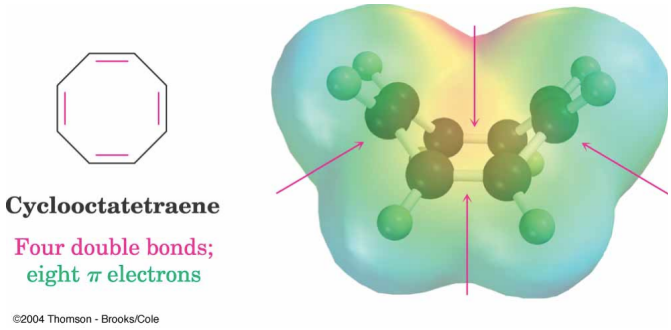




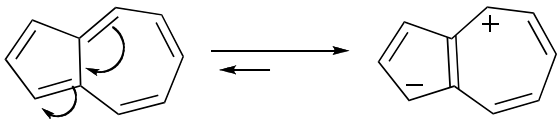
Special Compounds With 4n π Electrons



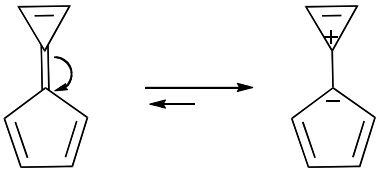
4π electrons
antiaromatic
Exists @ 4 K



Cool Aromatic Compounds



azulene

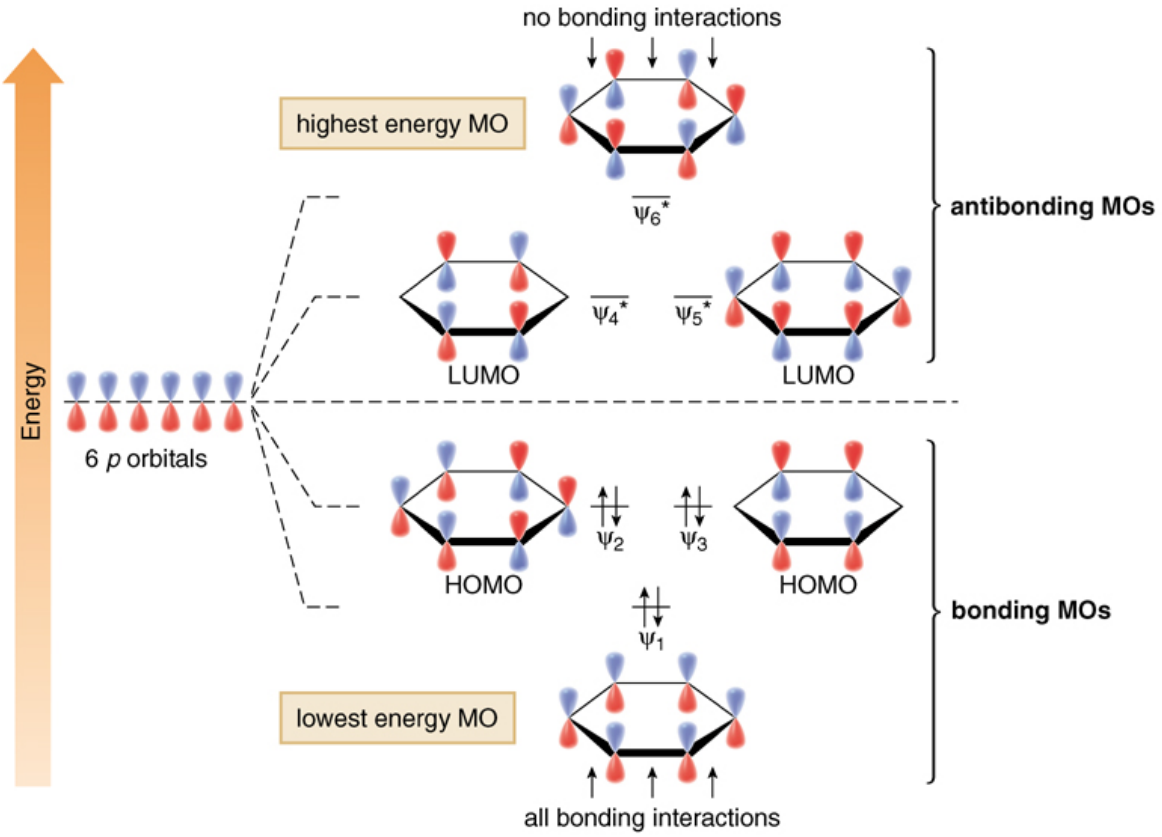


- Aromatic compounds composed smaller rings other than benzene are called **nonbenzenoid** aromatic compounds

Reactions at the Benzylic Carbon and Reductions of Aromatic Compounds

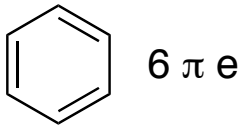
Oxidation with H_2CrO_4 or $KMnO_4$ (No Mechanism)
Free radical reactions (Review Mechanism)
SN_1, SN_2, E_1, E_2 (Review Mechanisms)
Hydrogenation (No arrow pushing Mechanism)
Birch reduction (Na, NH_3) with EWG and EDG

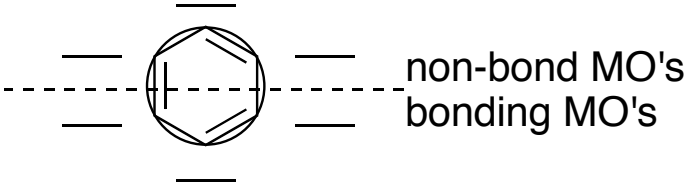
What is Aromaticity?

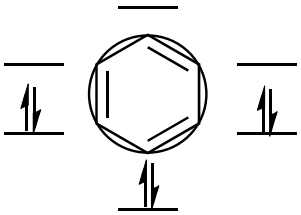


Frost Diagrams

1. Inscribe the ring in a concentric circle with one of the points down
2. Draw energy levels at each of the intersections between the circle and the ring
3. Cut circle in half
4. Fill the levels with π electrons starting at the bottom and working your way up

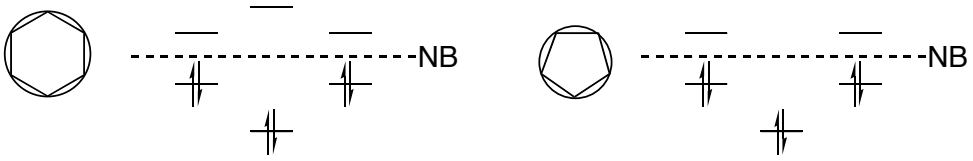




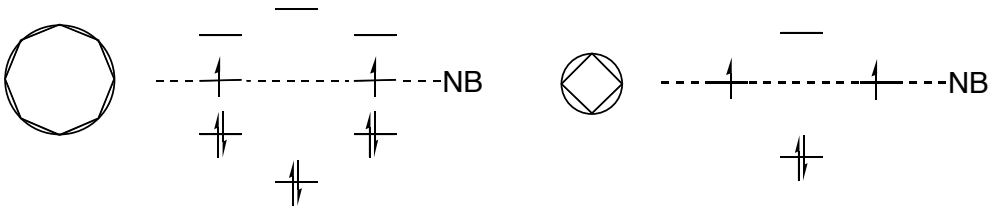


Why 4n+2?

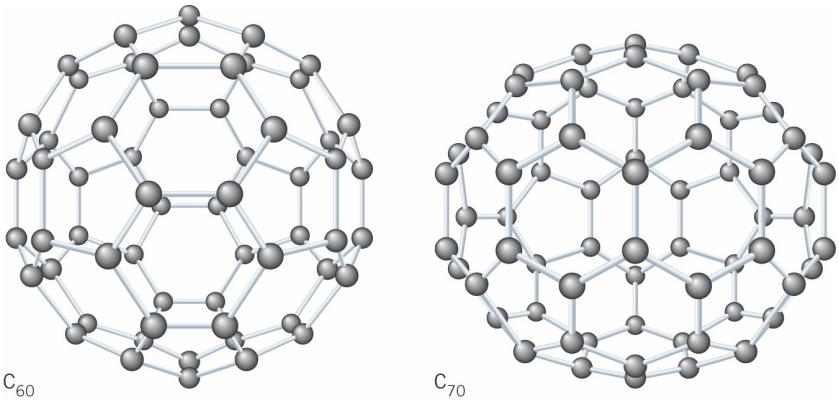
- Aromatic



- Antiaromatic or Nonaromatic



Fullerenes



- Bucky Balls
- A third allotrope of carbon
- Not aromatic because not planar and undergoes addition reactions