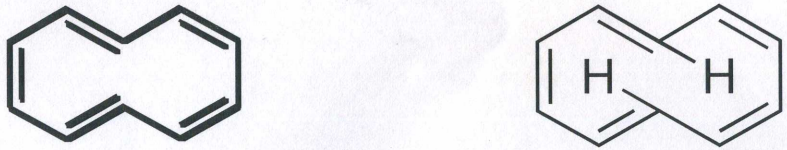
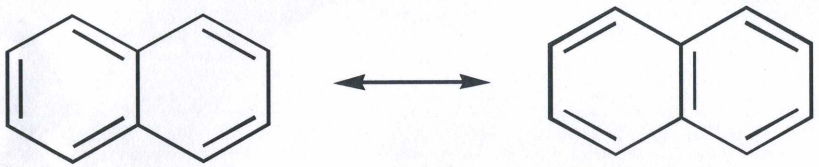
Aromaticity

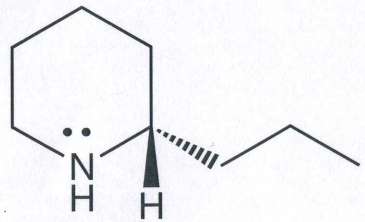


Cyclodecapentaene
Has 10 π electrons and fits 4n+2 rule for n=2 , but is not planar = not aromatic

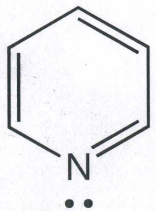


Naphthalene
Has 10 π electrons and fits 4n+2 rule for n=2 , is planar = aromatic

Heterocycles: have atoms other than C in ring, some are aromatic

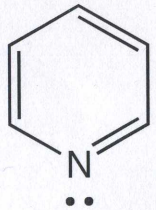


Coniine Non-aromatic heterocycle

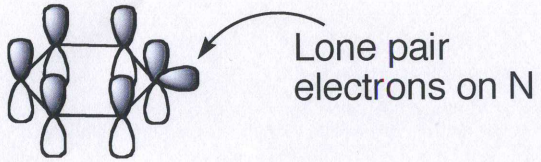


Pyridine aromatic heterocycle

Aromatic Heterocycles

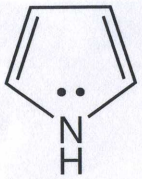


Pyridine

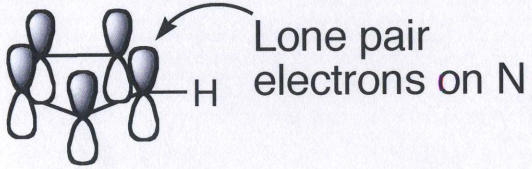


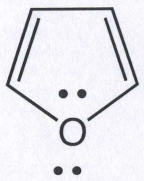
Pyridine is aromatic
Has 6 π electrons

molecules will be aromatic if they can as it imparts stability

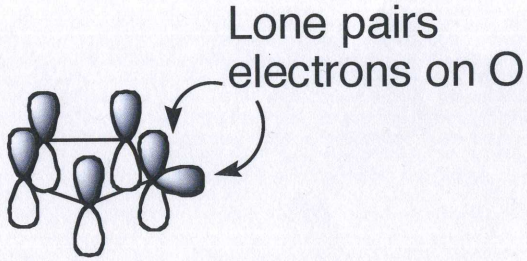


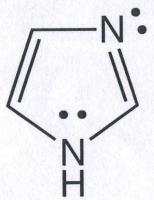
Pyrrole



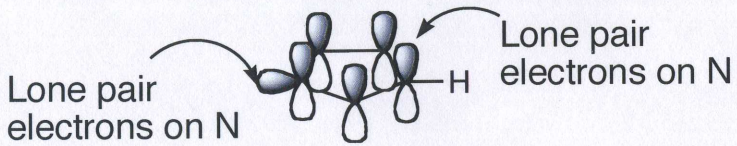


Furan



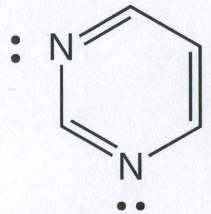


Imidazole

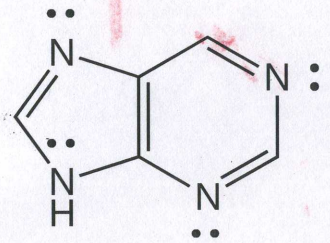


Aromatic Heterocycles and Ions

molecules will be aromatic if they can as it imparts stability: more examples



Pyrimidine

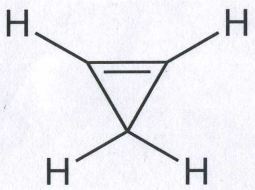


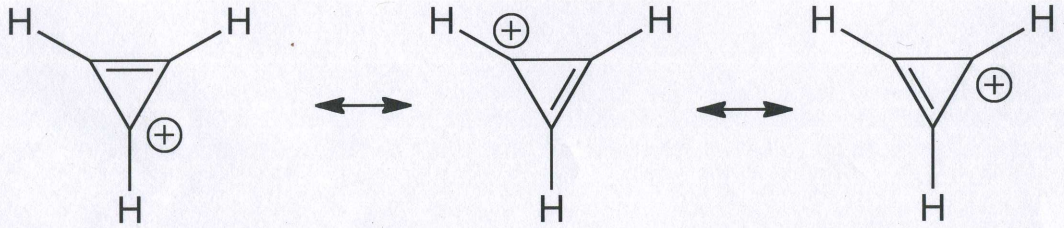
Purine

Aromatic intermediates: cations and anions

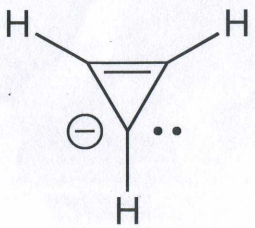
cyclopropane and cyclopropene are extremely reactive - due to angle strain

but cyclopropene cation is more stable than expected (still very reactive)



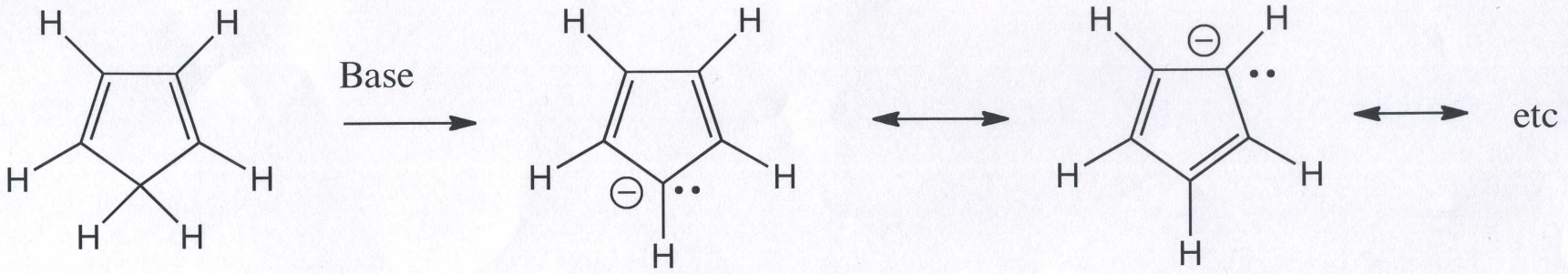


aromatic cation : has 2 π electrons (4n+2, n=0)



anion not aromatic : has 4 π electrons

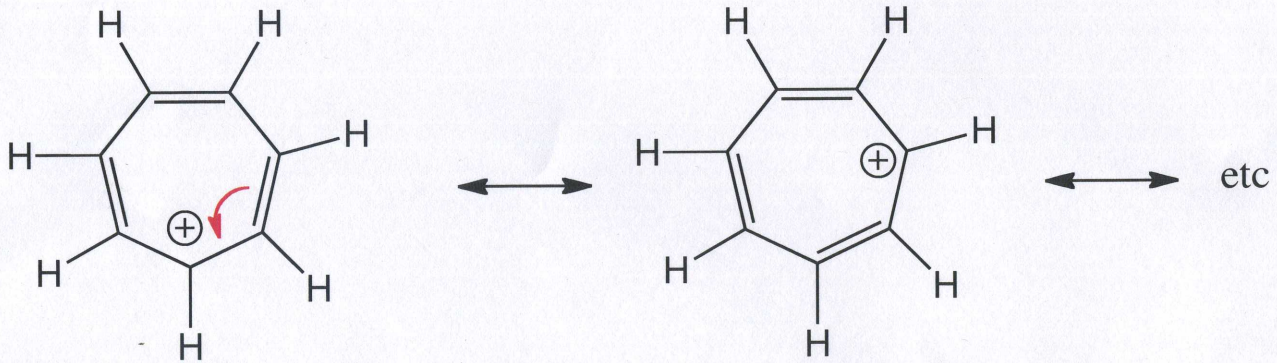
Aromatic Ions



cyclopentadiene
pKa = 16 !

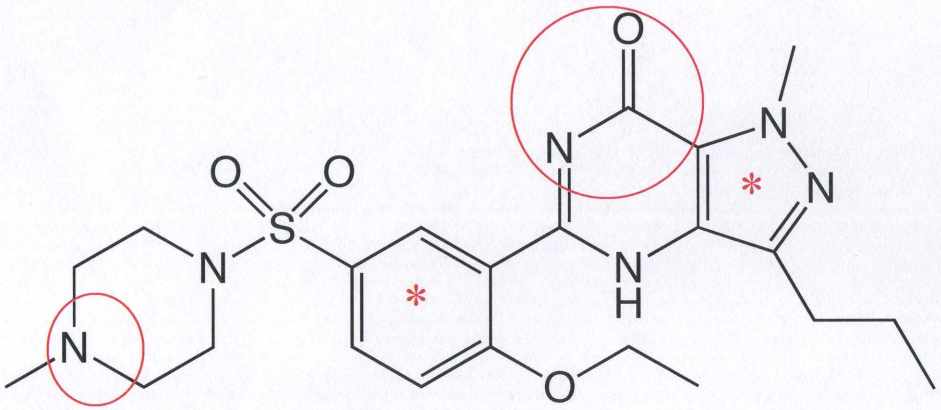
aromatic anion : has 6 π electrons (4n+2, n=1)

acidity of cyclopentadiene hydrogen enhanced by 30 orders of magnitude (30 pKa units



cycloheptatrienyl cation aromatic : has 6 π electrons

Some things you should know: functional groups & structure



Viagra: $2.3 B / yr

aids jet lag recovery in hamsters

Can you recognize its functional groups? (amine, amide)

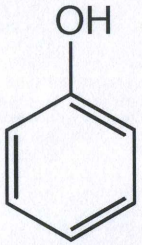
Molecular formula ? ($C_{22}H_{30}N_6O_4S$)

Which rings are aromatic ? (*)

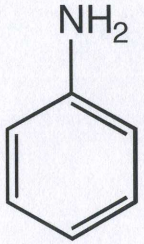
Stereogenic centers? (No)

Nomenclature of Aromatic Compounds

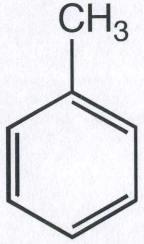
Common Substituted Benzene Structures (that you should know):



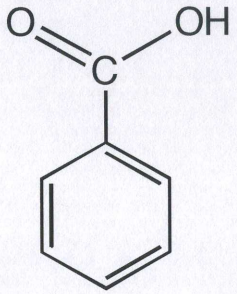
Phenol



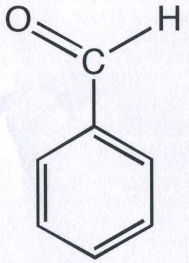
Aniline



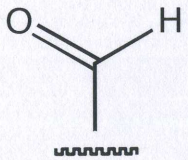
Toluene



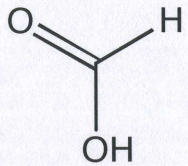
Benzoic Acid



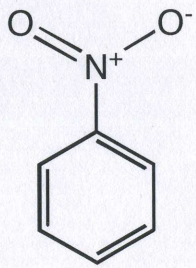
Benzaldehyde



An Aldehyde Group
aka Formyl Group



Formic Acid



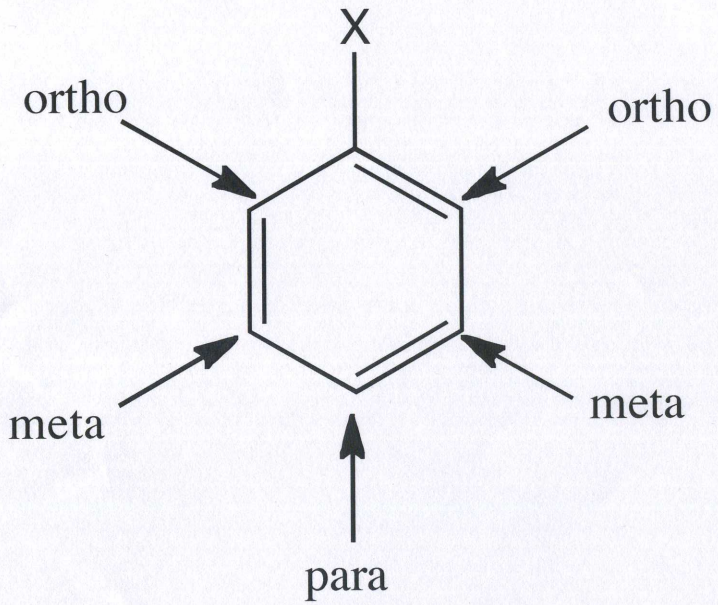
Nitrobenzene

NO_2 is a
nitro group

Nomenclature of Aromatic Compounds

Nomenclature of substituted benzene rings

with 2 substituents on a benzene ring, *ortho*, *meta*, and *para* are used to indicate position (or relative position)



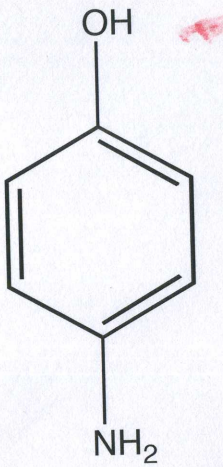
Ortho refers to 1,2-substitution and is abbreviated o-

Meta refers to 1,3-substitution and is abbreviated m-

Para refers to 1,4-substitution and is abbreviated p-

Nomenclature of Aromatic Compounds

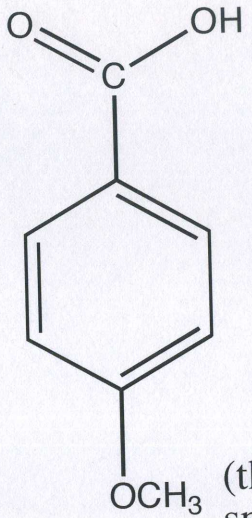
Examples



p-aminophenol
(more correct, OH has priority)

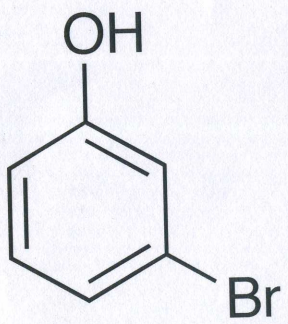
or

p-hydroxyaniline



p-methoxybenzoic acid

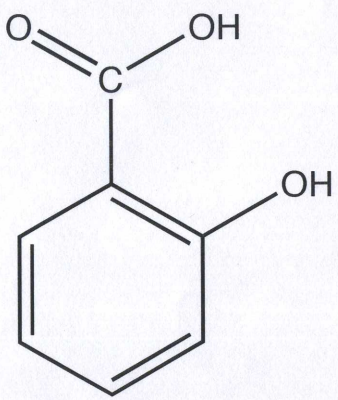
(this is an ether group, specifically methoxy)



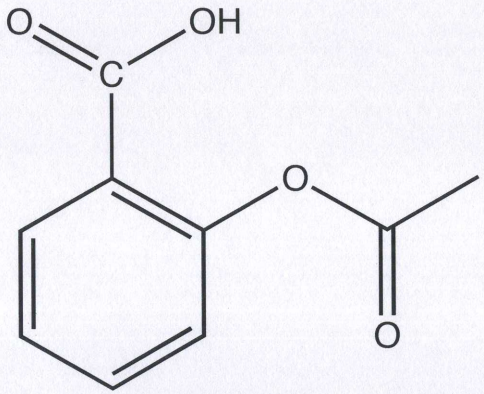
m-bromophenol or meta-bromophenol or 3-bromophenol

Nomenclature of Aromatic Compounds

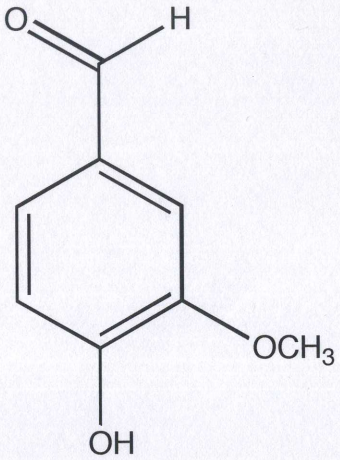
Examples



2-hydroxybenzoic acid
(salicyclic acid)



2-acetoxybenzoic acid
acetylsalicylic acid
(aspirin)



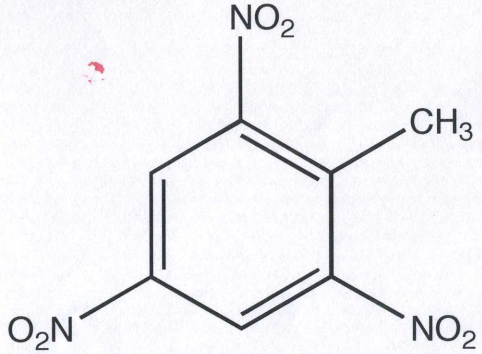
4-hydroxy-3-methoxybenzaldehyde
(or vanillin)

The carbon substituent (an aldehyde or acid group) usually gets priority

Then number the ring such that the substituents have the lowest numbers

Nomenclature of Aromatic Compounds

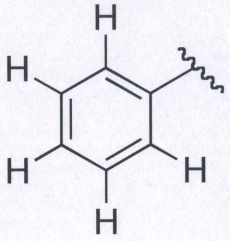
Example



2,4,6-trinitrotoluene (TNT)

Aromatic Groups:

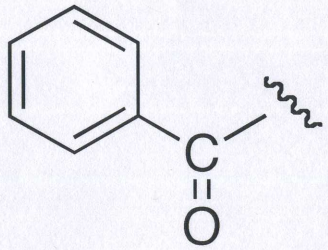
Ph ≡ ϕ ≡

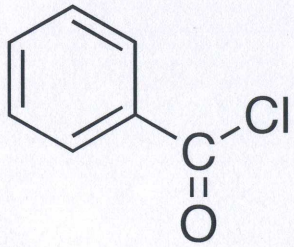


Phenyl group

Ar = aryl = any aromatic group

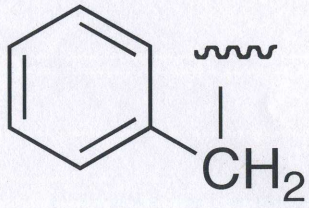
Bz = benzoyl group

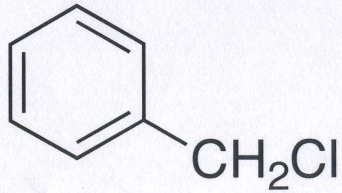




benzoyl chloride

Bn = benzyl group

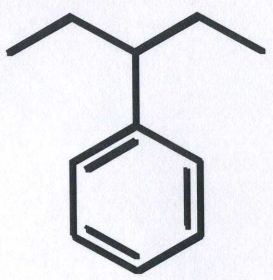




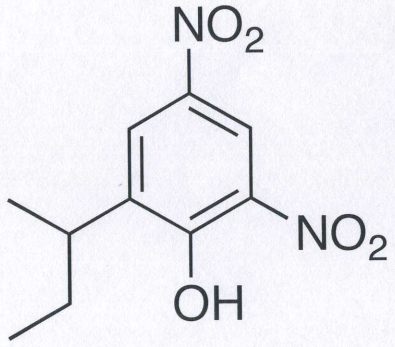
benzyl chloride

Nomenclature of Aromatic Compounds

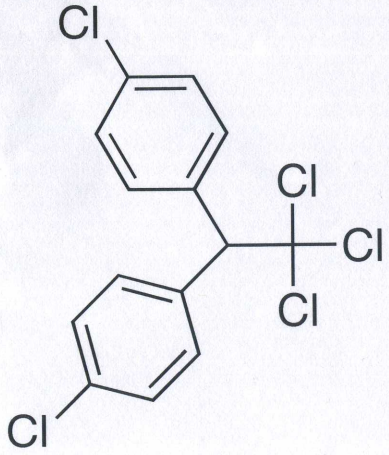
sometimes useful to name a compound with the aromatic part as a substituent



3-phenylpentane



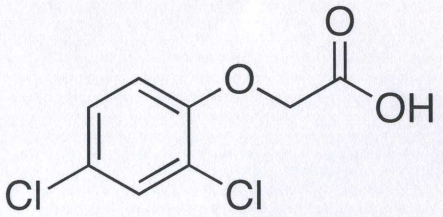
2-*sec*-butyl-4,6-dinitrophenol
(Amaize) a corn yield enhancer
6-(1-methylpropyl)-2,4-dinitrophenol



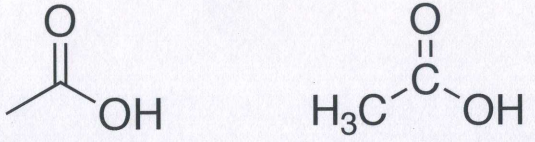
DDT - an insecticide - to wipe out malarial mosquito
Paul Muller won 1948 Nobel Prize in Medicine for it

1,1,1-trichloro-2,2-bis-(4-chlorophenyl)ethane

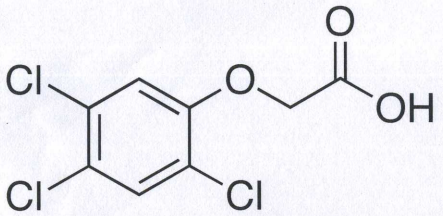
Nomenclature of Aromatic Compounds



2,4-D 2,4-dichlorophenoxyacetic acid



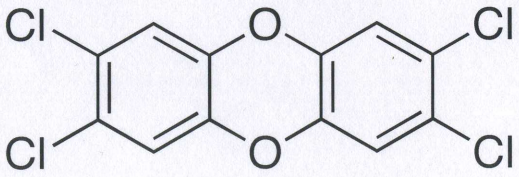
acetic acid



2,4,5-T 2,4,5-trichlorophenoxyacetic acid

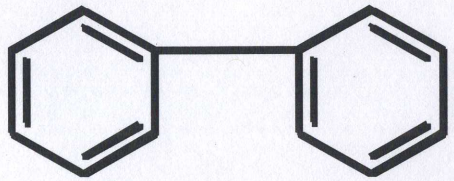
Agent Orange

Weed and Feed

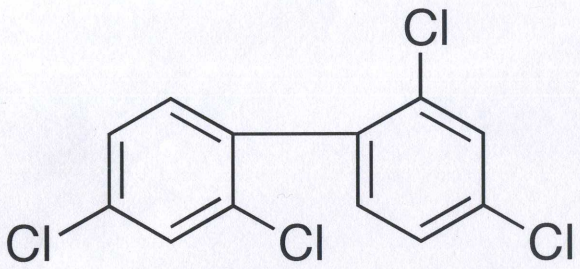


dioxin

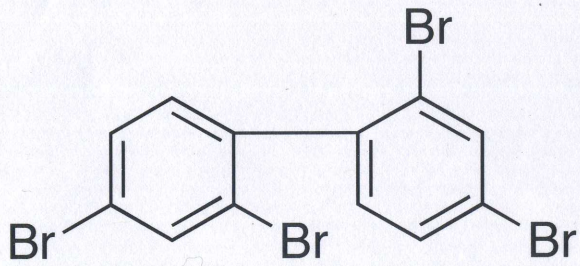
Nomenclature of Aromatic Compounds



biphenyl



a polychlorinated biphenyl PCB



a polybrominated biphenyl PBB