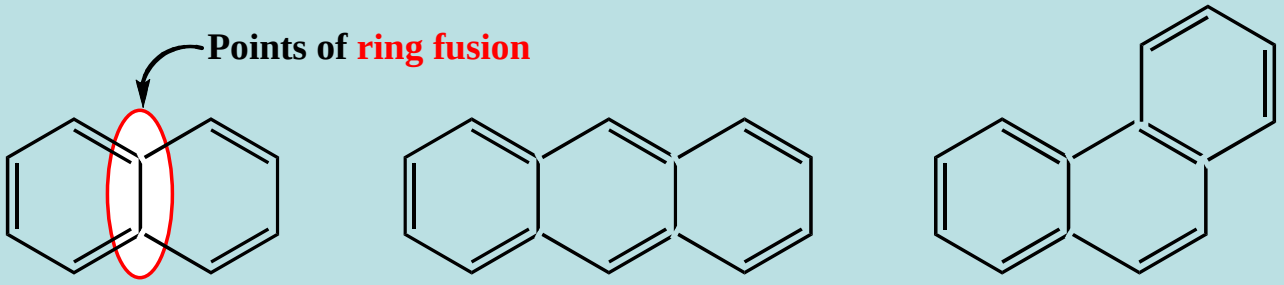
Polynuclear Benzenoid Aromatic Compounds

Many compounds are known that have two or more benzene rings "fused" together. These compounds are called polynuclear aromatic compounds.



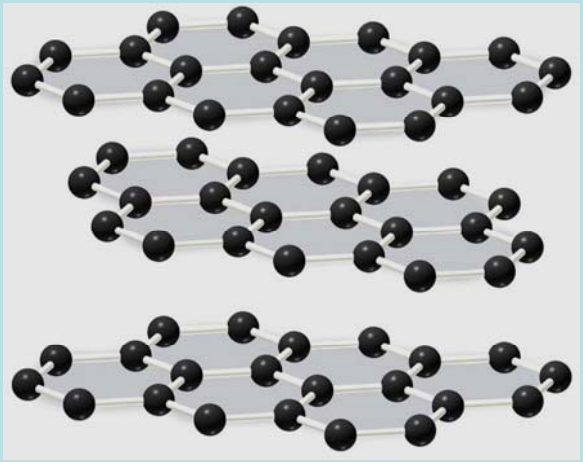
Naphthalene $C_{10}H_8$

Anthracene $C_{14}H_{10}$

Phenanthrene $C_{14}H_{10}$

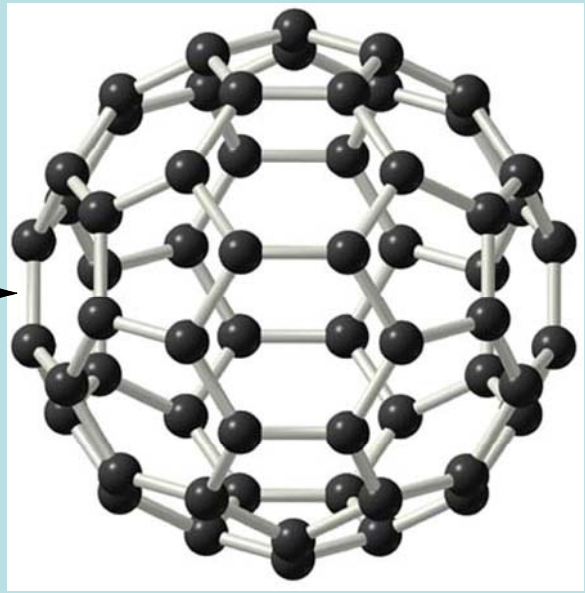
These structures are planar with continuous overlap of the p-orbitals. Calculations and heat of hydrogenation data indicate considerable stabilization energy in these compounds.

Graphite, Fullerenes and Nanotubes



High temper-ature

Inert atmos-phere



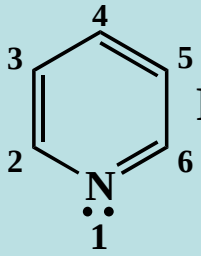
Nature of graphite arrays (parallel planar sheets of sp^2-type carbon atoms)

C_{60} Fullerene (consists of slightly non-planar arrays of sp^2-type carbon atoms)

Nanotubes are related structures, two half fullerene units separated by a cylinder that may be thought of as a rolled graphite sheet.

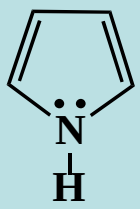
These spheres and tubes have great stability, retaining this characterisic of aromaticity in spite of their bent sp^2 carbon bonding.

Some Heterocyclic Aromatic Compounds

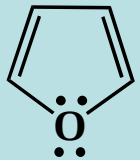


Pyridine, a nitrogen-containing analog of benzene

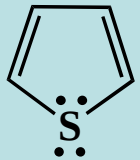
[Note that in cyclic compounds a heteroatom is always assigned ring number 1.]



Pyrrole

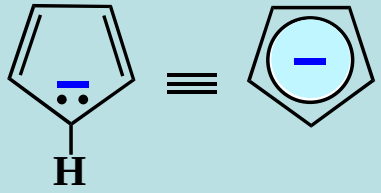


Furan



Thiophene

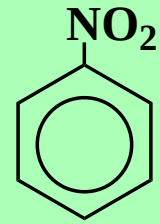
Hetero analogs of cyclopentadienyl anion:



Quiz 14.01

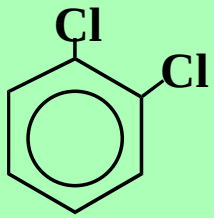
Assign names for aromatic compounds A through E using the provided information (in blue).

A



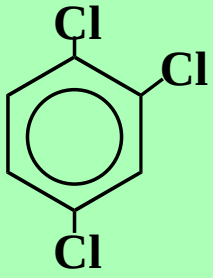
Nitrobenzene

B

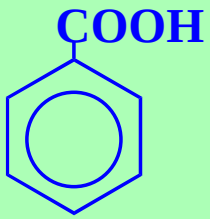


1,2-Dichlorobenzene or
ortho-Dichlorobenzene

C

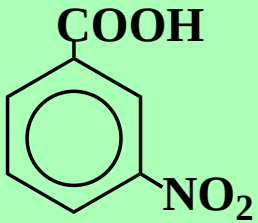


1,2,4-Trichlorobenzene

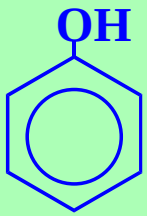


Benzoic acid

D

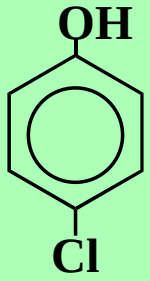


3-Nitrobenzoic acid or
meta-Nitrobenzoic acid



Phenol

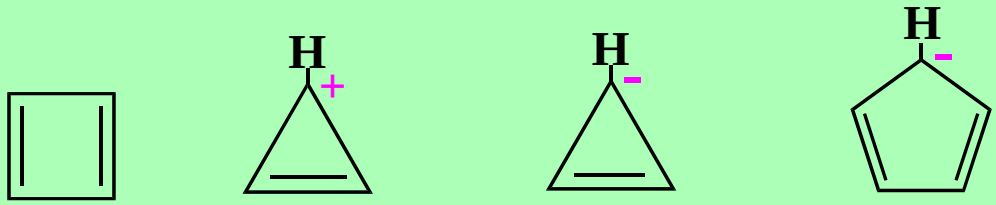
E



4-Chlorophenol or
para-Chlorophenol

Quiz 14.03

Use the polygon-and-circle method to predict which of the the following species is aromatic or non-aromatic.

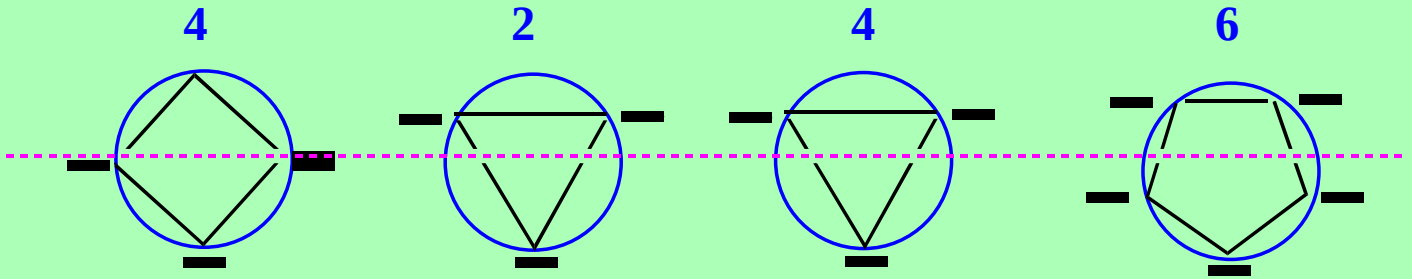


Solution:

Determine the number of π electrons in each system.

Inscribe the polygon inside a circle (corner down) and find the levels of the π molecular orbitals. Then fill them, starting with the lowest energy MO. Determine if the π electrons all lie in MO's that are stabilized.

Number of π electrons:



non-aromatic **aromatic** **non-aromatic** **aromatic**