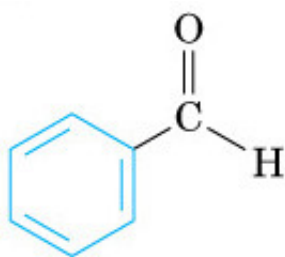


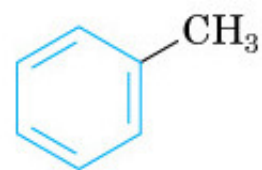
Sistemi aromatici



Benzene



Benzaldeide



Toluene

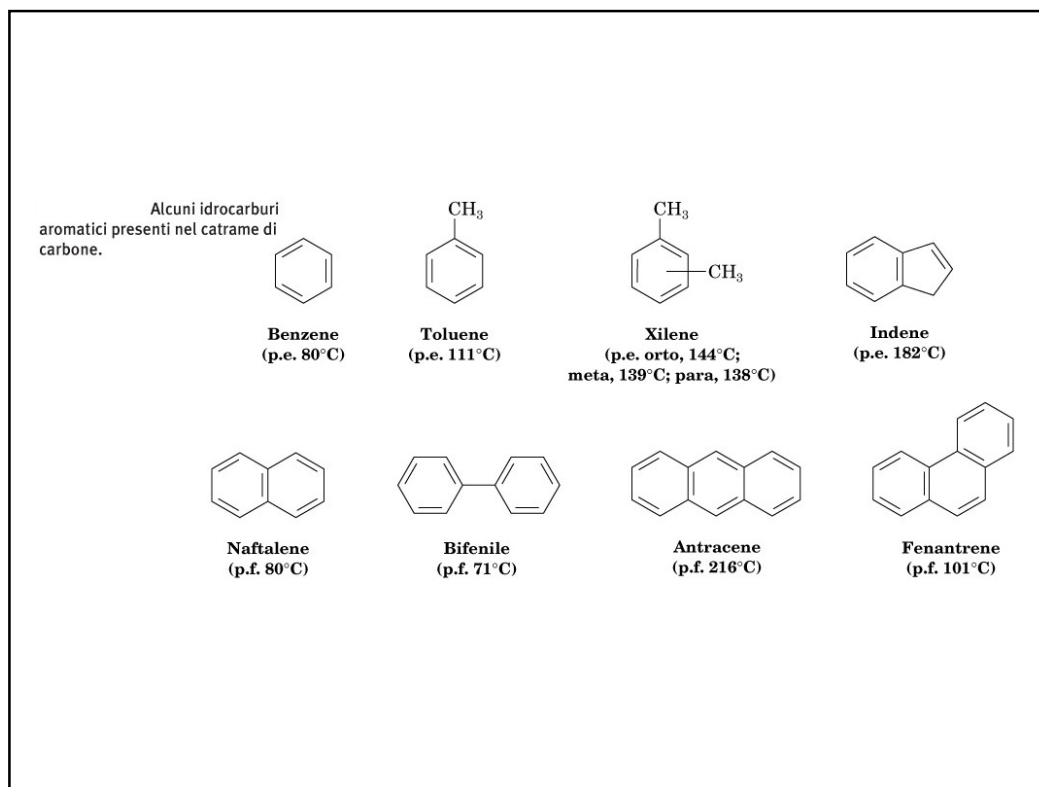
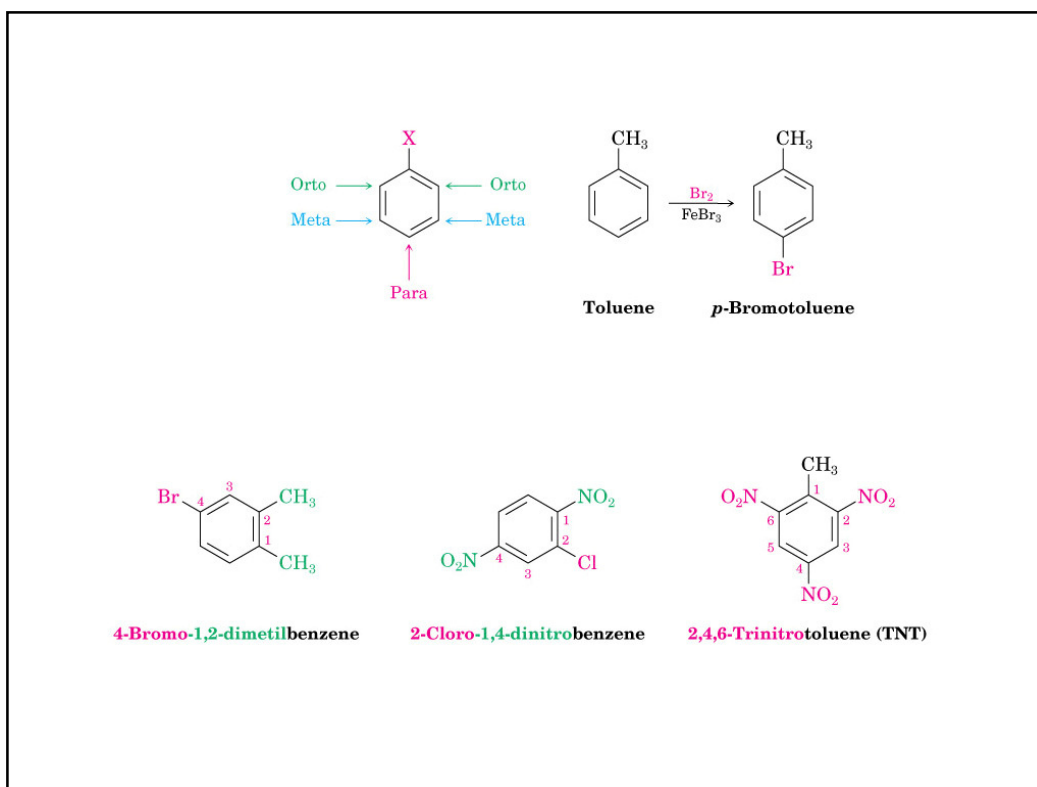
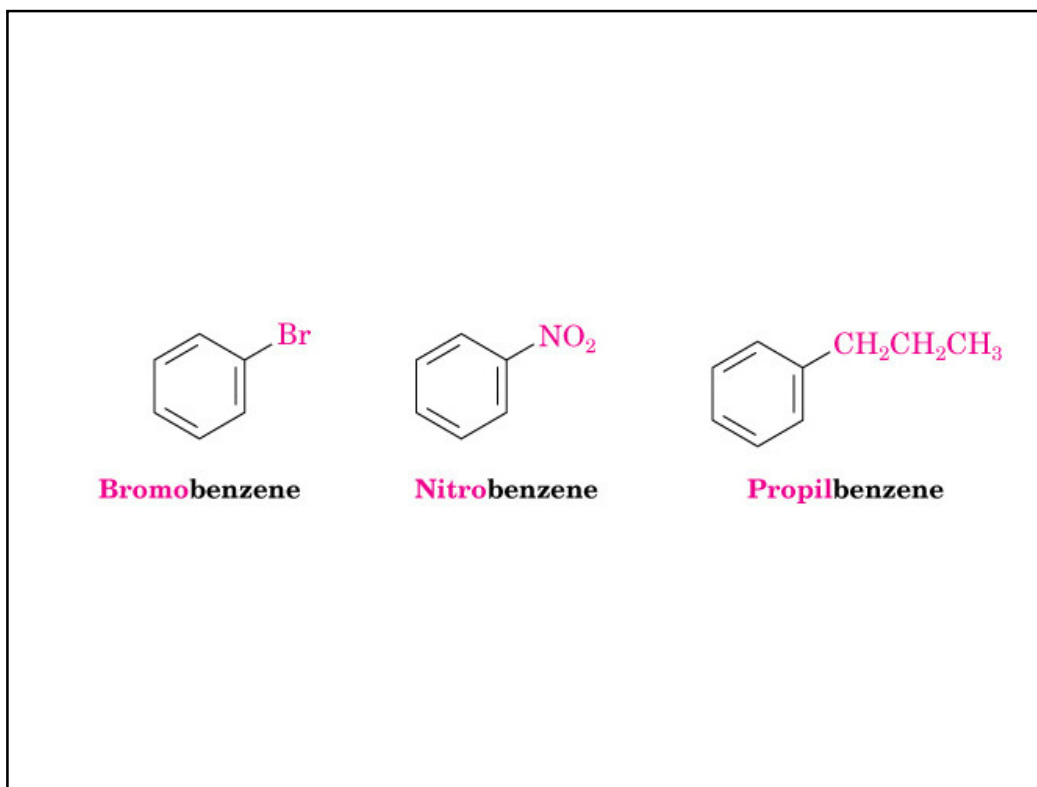
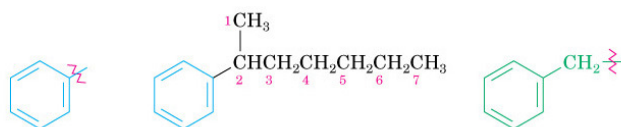


TABELLA 15.1 Nomi comuni di alcuni composti aromatici

Formula	Nome	Formula	Nome
	Toluene (p.e. 111°C)		Benzaldeide (p.e. 178°C)
	Fenolo (p.f. 43°C)		Acido benzoico (p.f. 122°C)
	Anilina (p.e. 184°C)		Benzonitrile (p.e. 191°C)
	Acetofenone (p.f. 21°C)		orto-Xilene (p.e. 144°C)
	Cumene (p.e. 152°C)		Stirene (p.e. 145°C)



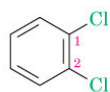
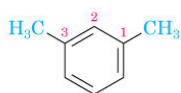
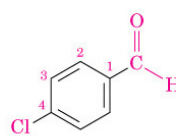


Gruppo fenilico

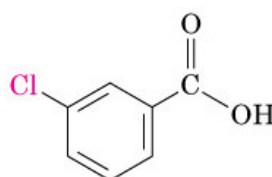
2-Fenileptano

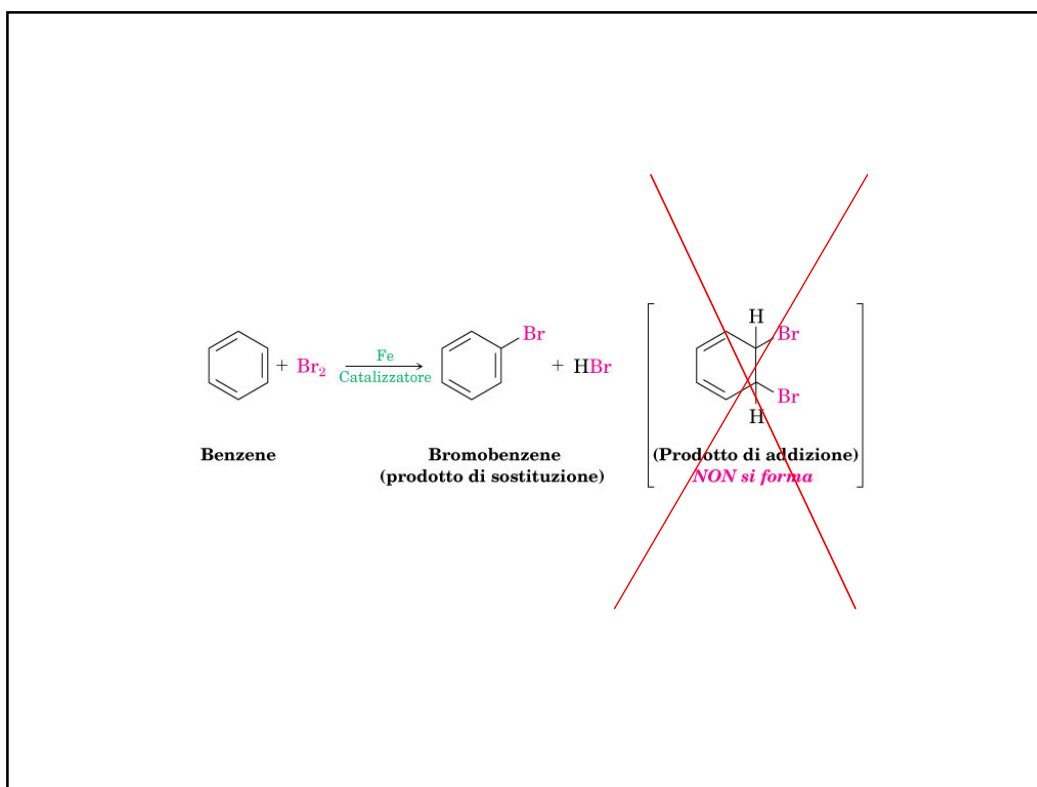
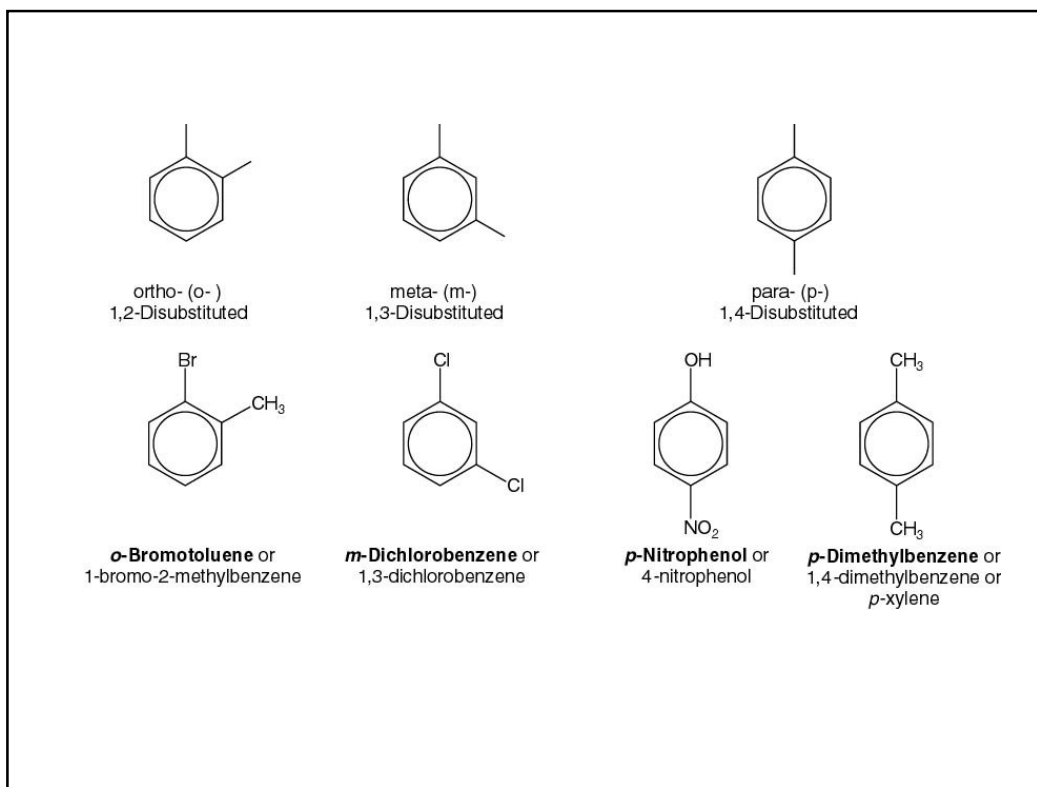
Gruppo benzilico

I benzene disostituiti vengono denominati usando i prefissi *orto-* (*o*), *meta-* (*m*), o *para-* (*p*). Un benzene orto-disostituito porta i due sostituenti nell'anello in posizione 1,2, un benzene meta-disostituito ha i due sostituenti in posizione 1,3, e un benzene para-disostituito presenta i sostituenti in posizione 1,4.

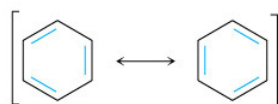
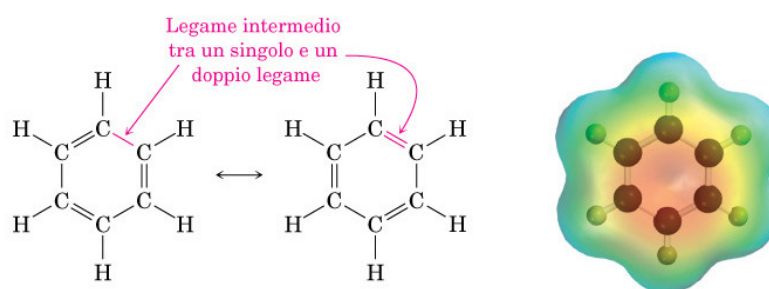
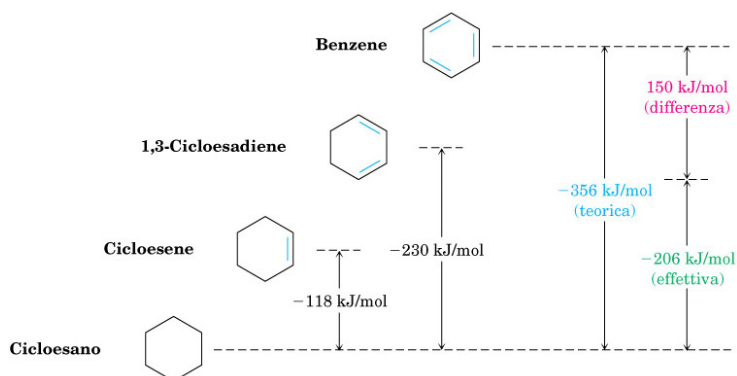
*orto*-Diclorobenzene
1,2 disostituito*meta*-Xilene
1,3 disostituito*para*-Clorobenzaldeide
1,4 disostituito

2,6-Dibromofenolo

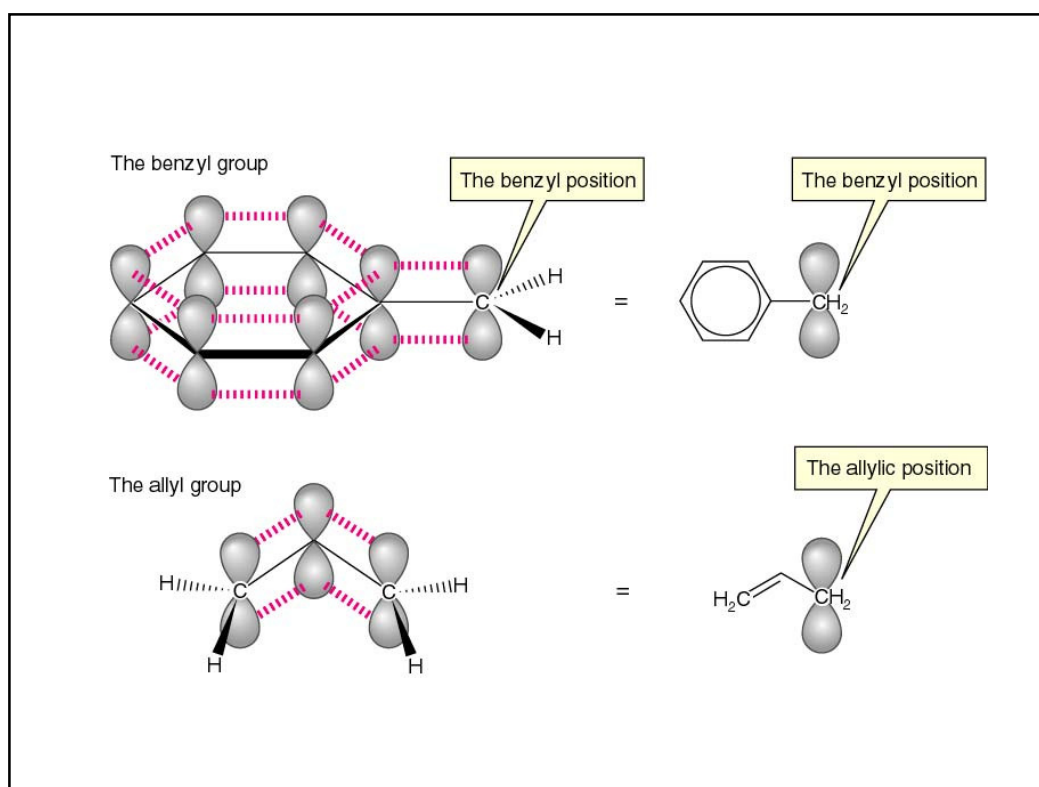
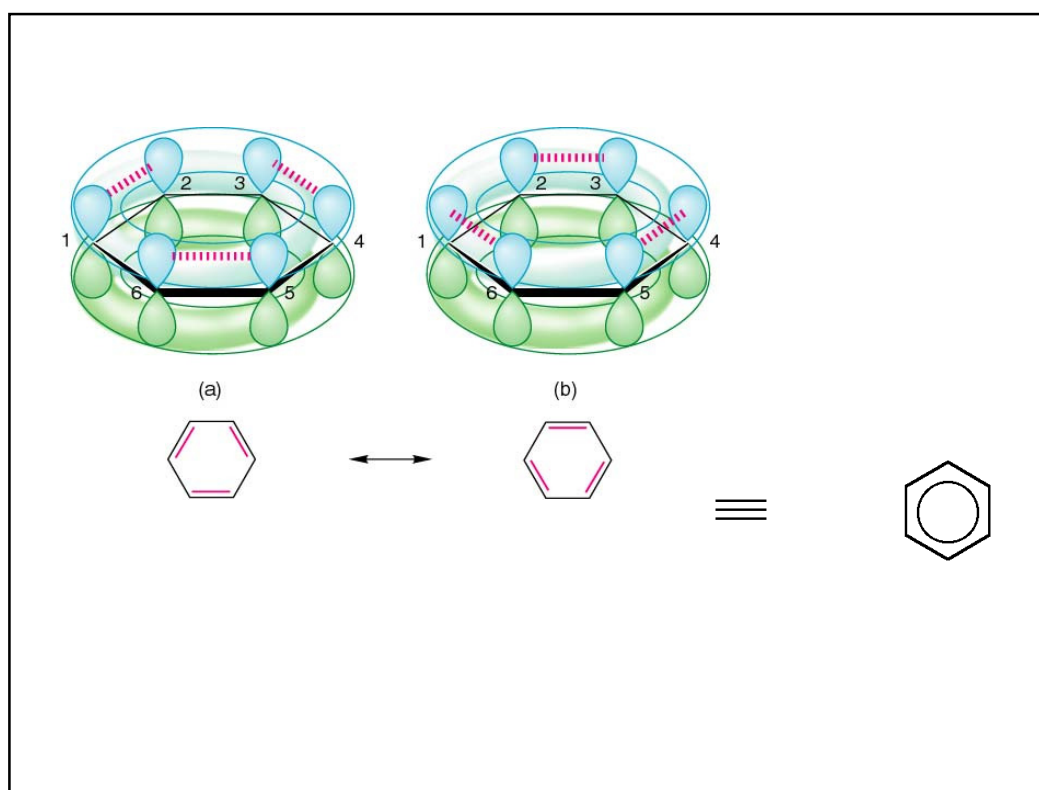
Acido *m*-clorobenzoico



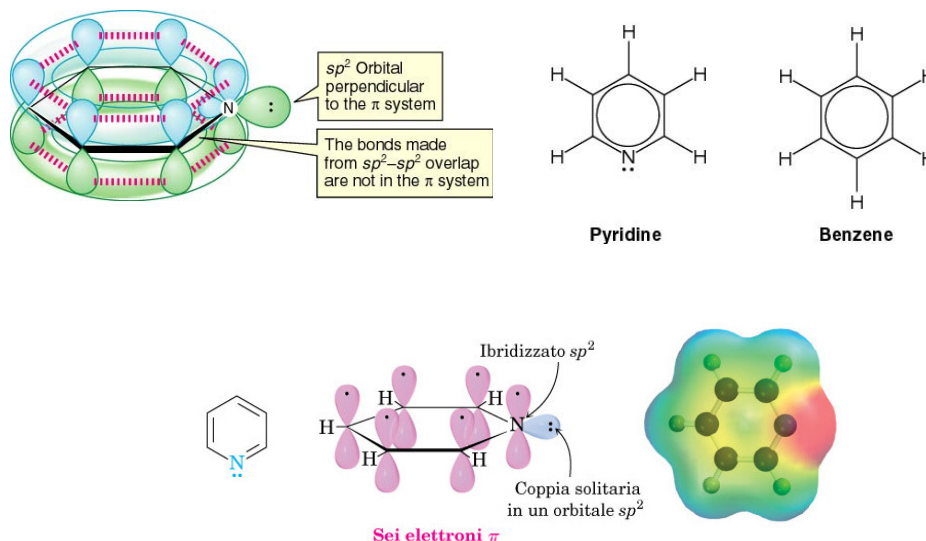
Confronto dei calori di idrogenazione per il cicloesene, 1,3-cicloesadiene e benzene. Il benzene risulta di 150 kJ/mole (36 kcal/mol) più stabile di quanto ci si potrebbe aspettare per il “cicloesatriene”.



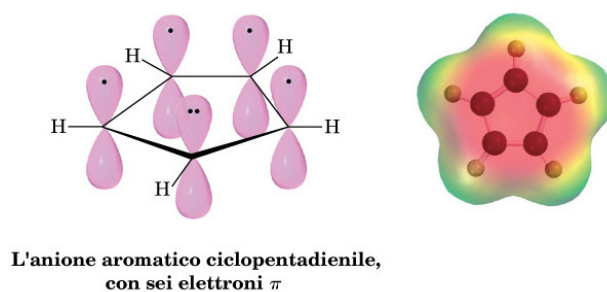
Rappresentazioni alternative del benzene. La rappresentazione con il cerchio deve essere usata con attenzione dal momento che non indica in numero degli elettroni π nell'anello.

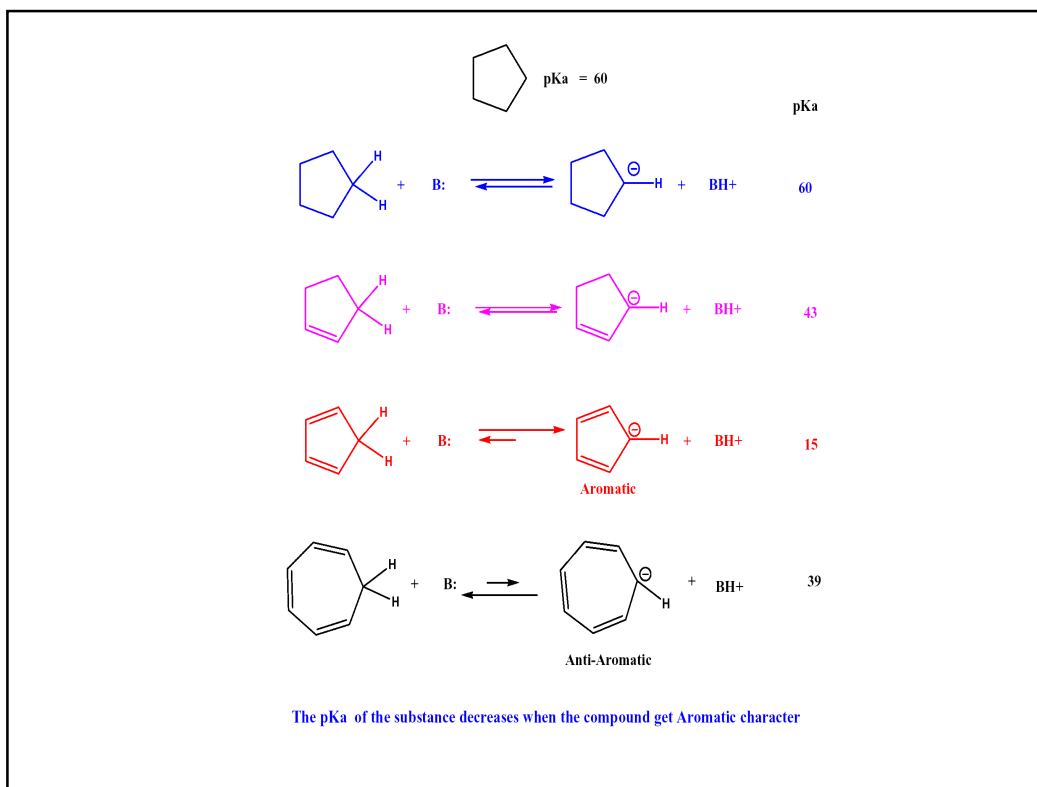


Sistemi eteroaromatici

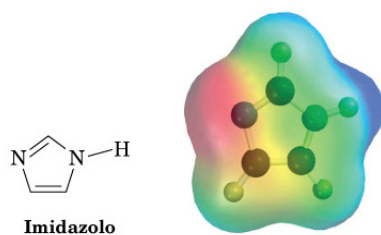
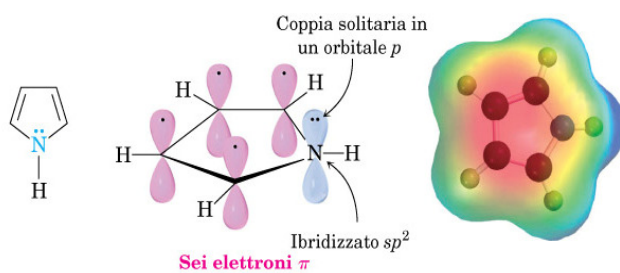


Rappresentazione degli orbitali dell'anione ciclopentadienile che dimostra la coniugazione ciclica dei sei elettroni p nei cinque orbitali p. La mappa di potenziale elettrostatico indica che lo ione risulta simmetrico, e che tutti i cinque atomi di carbonio sono elettronricchi (rosso).



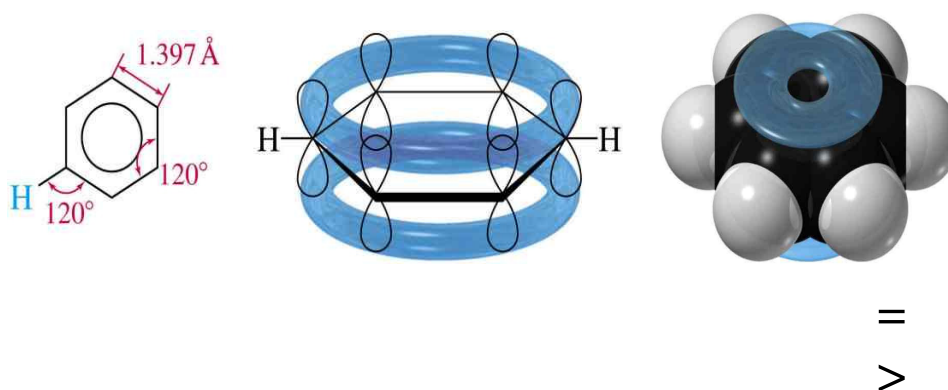


Il pirrolo, un eterociclo aromatico a cinque termini, ha una disposizione degli elettroni p molto simile a quella dell' anione ciclopentadienile.

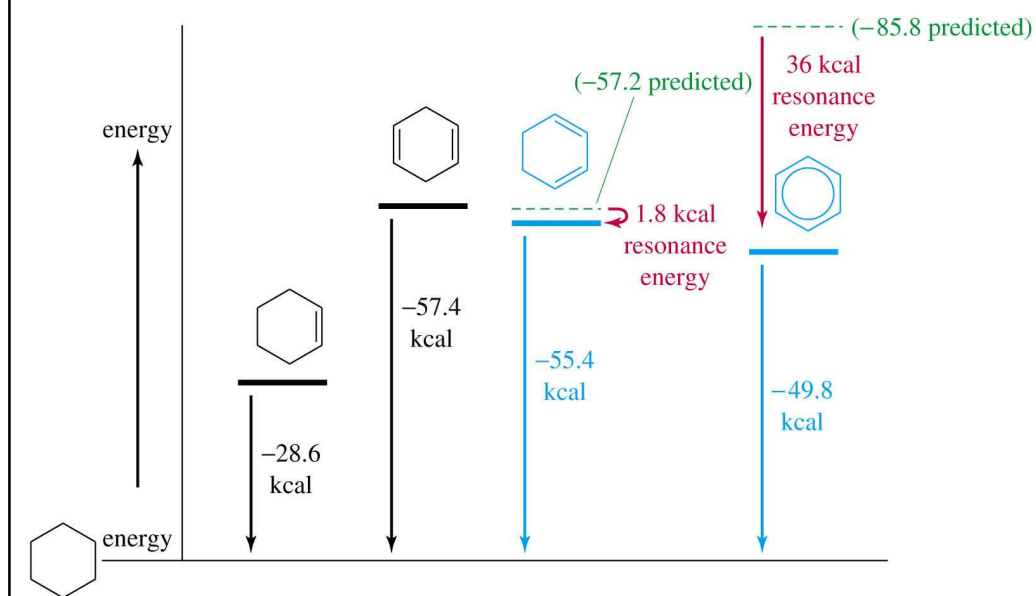


Resonance Structure

Each sp^2 hybridized C in the ring has an unhybridized p orbital perpendicular to the ring which overlaps around the ring.

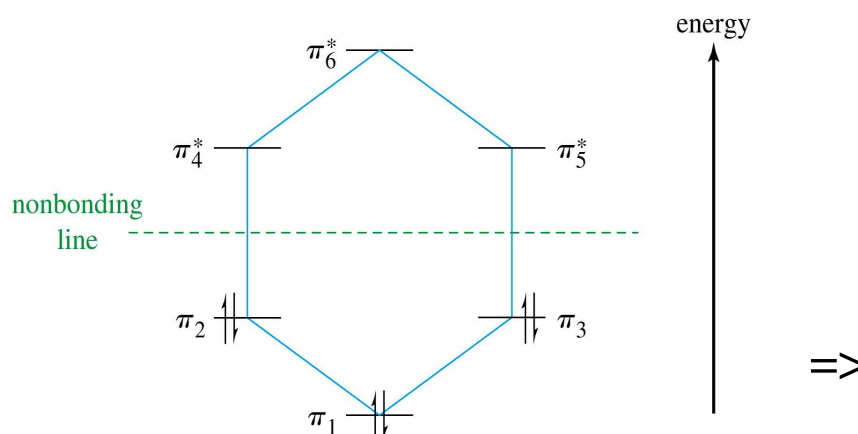


Unusual Stability



Energy Diagram for Benzene

- The six electrons fill three bonding pi orbitals.
- All bonding orbitals are filled (“closed shell”), an extremely stable arrangement.



◆ Le molecole sono aromatiche se sono soddisfatte le seguenti condizioni:

- ◆ La molecola è ciclica
- ◆ La molecola è interamente coniugata
- ◆ La molecola è planare (atomi di carbonio con ibridazione sp^2)
- ◆ regola di Hückel: la molecola contiene $(4n + 2)$ elettroni- π (con $n = 1, 2, 3, \dots$)

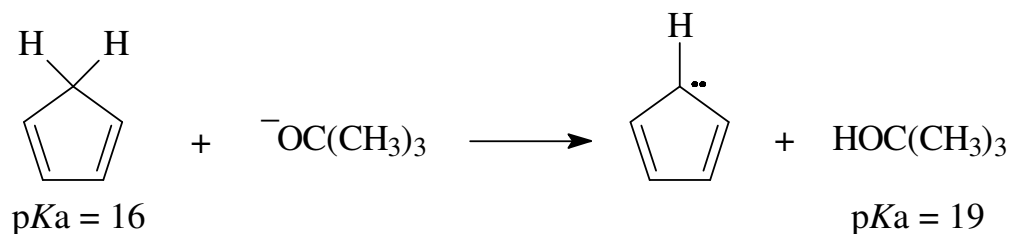
Hückel's Rule

- If the compound has a continuous ring of overlapping p orbitals and has $4N + 2$ electrons, it is aromatic.
- If the compound has a continuous ring of overlapping p orbitals and has $4N$ electrons, it is antiaromatic.

=>

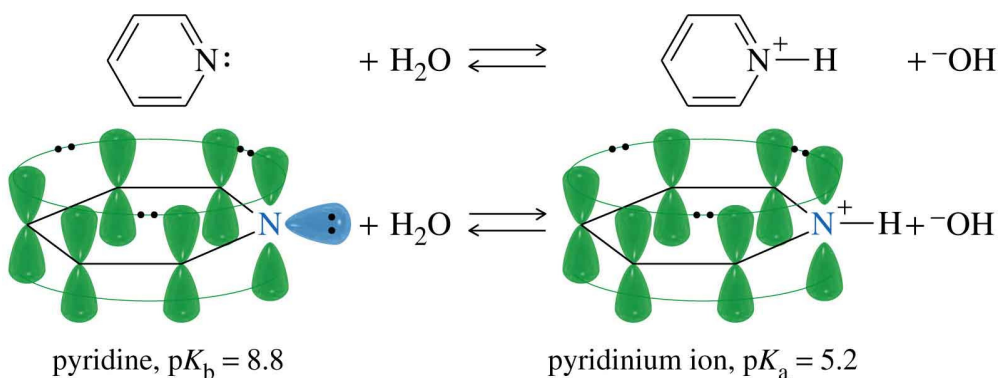
Acidity of Cyclopentadiene

pK_a of cyclopentadiene is 16, much more acidic than other hydrocarbons.



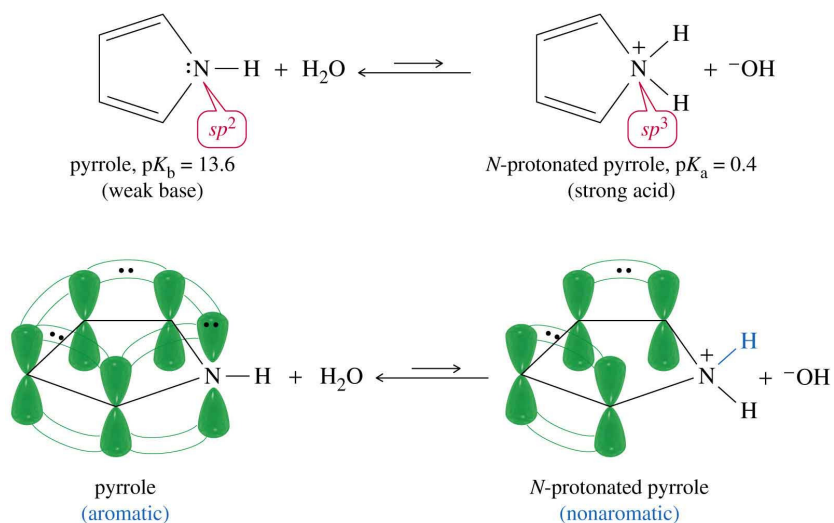
Pyridine

- Heterocyclic aromatic compound.
- Nonbonding pair of electrons in sp^2 orbital, so weak base, $pK_b = 8.8$.

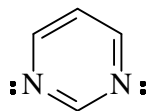


Pyrrole

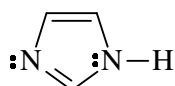
Also aromatic, but lone pair of electrons is delocalized, so much weaker base.



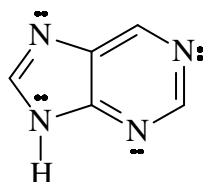
Basic or Nonbasic?



Pyrimidine has two basic nitrogens.

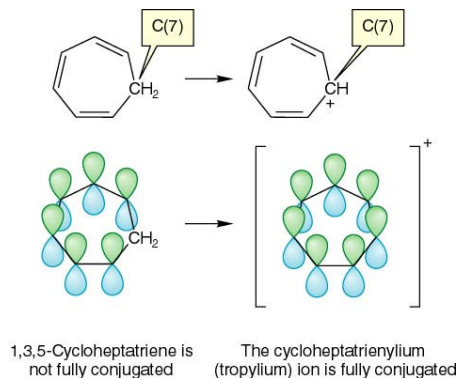
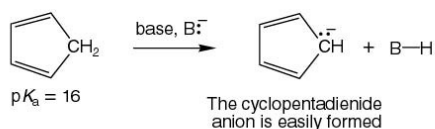


Imidazole has one basic nitrogen and one nonbasic.

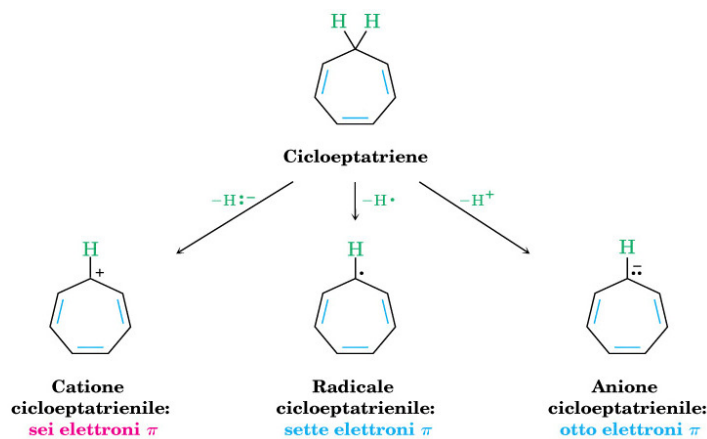


Purine?

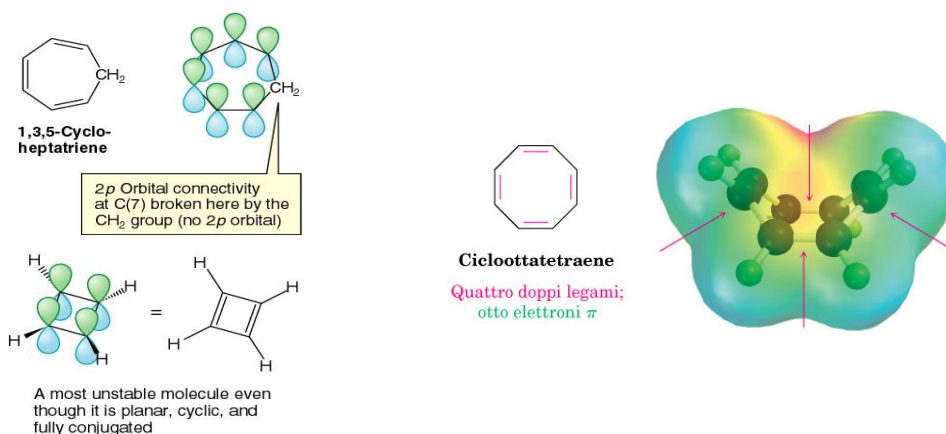
Composti aromatici

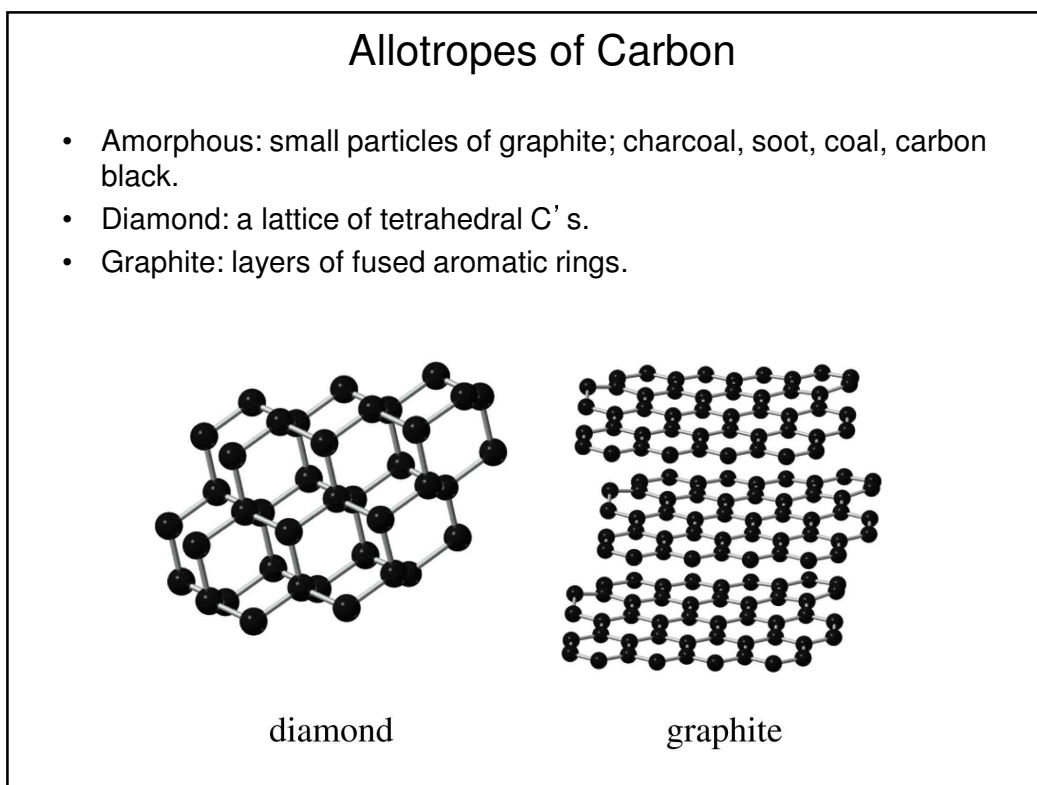
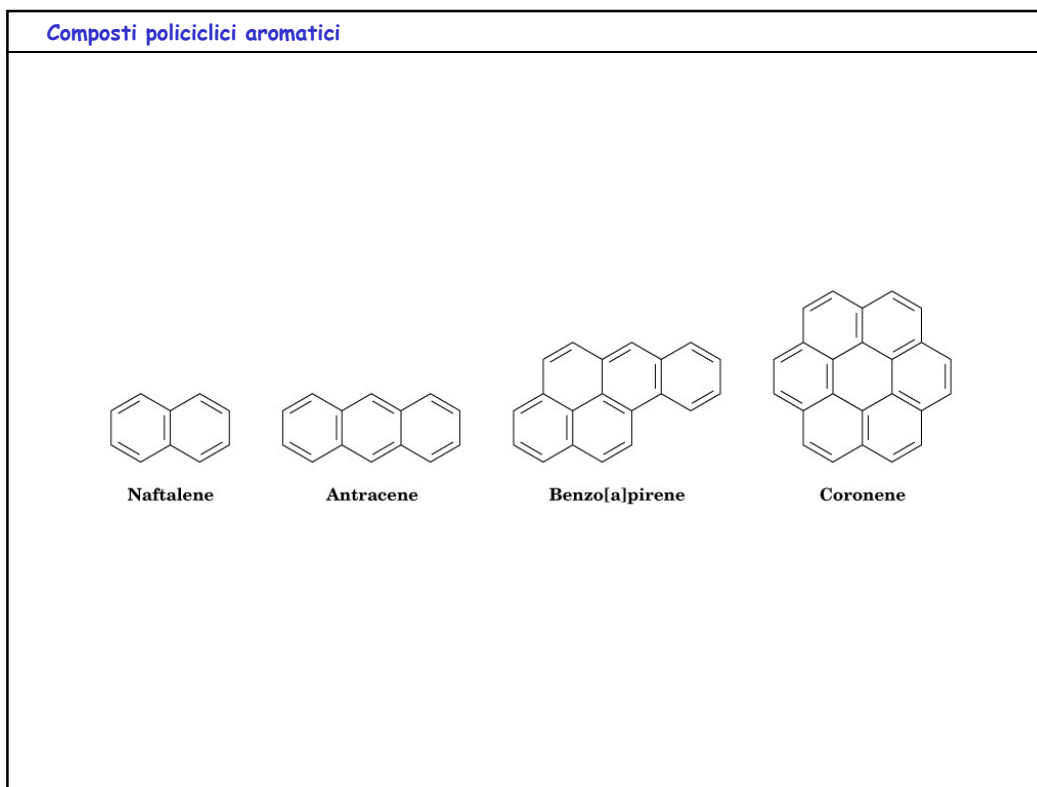


Formazione del catione, radicale e anione cicloeptatrienile.
Soltanto il catione a sei elettroni p risulta aromatico.



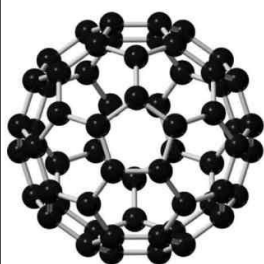
Composti Non-aromatici



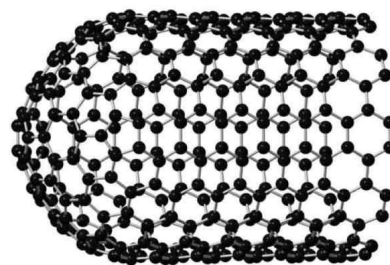
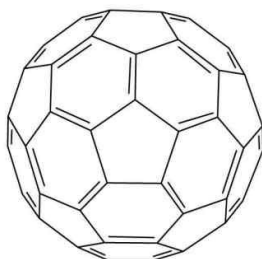


Some New Allotropes

- Fullerenes: 5- and 6-membered rings arranged to form a “soccer ball” structure.
- Nanotubes: half of a C_{60} sphere fused to a cylinder of fused aromatic rings.



buckyball (C_{60})



carbon nanotube