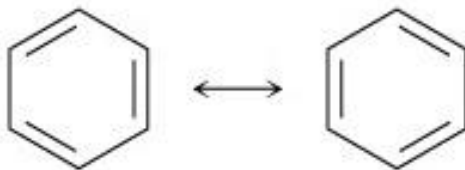
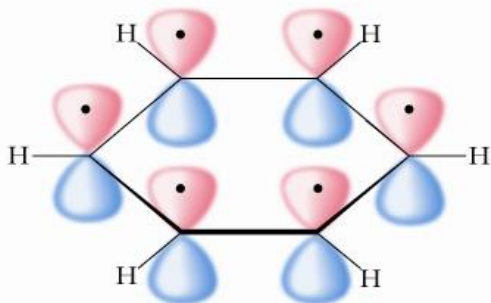
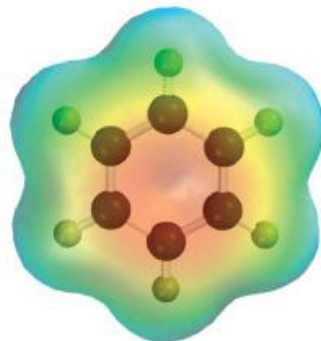
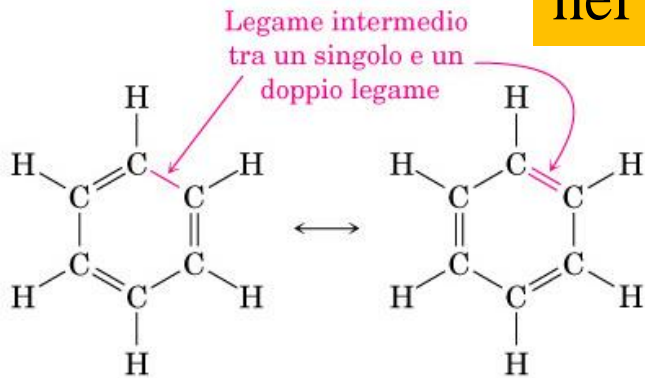


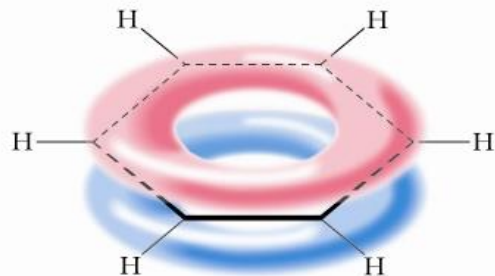
Benzene e aromaticità



Doppi legami coniugati nel benzene

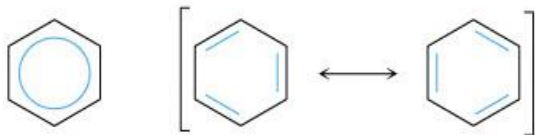


(a)



(b)

Risonanza del benzene



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.

Requisiti per l'aromaticità:

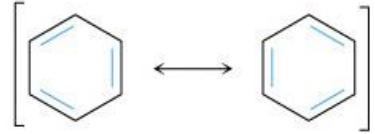
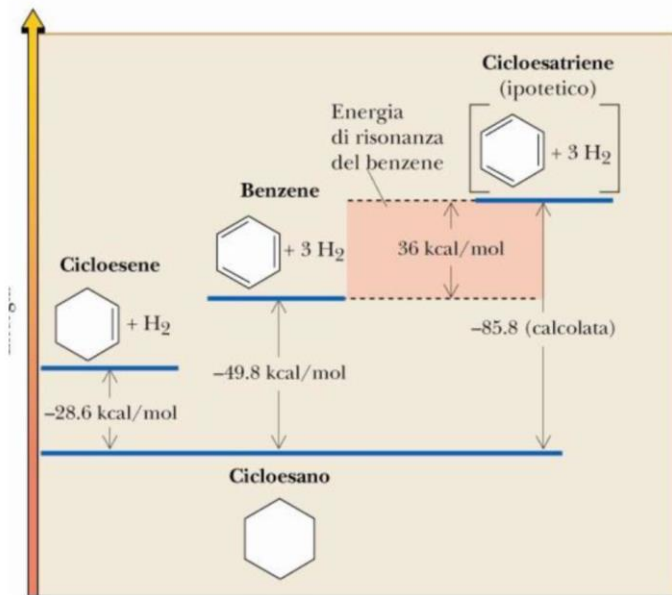
Molecola ciclica

Planare

atomi ibridizzati sp^2

Sistema coniugato continuo di elettroni contenete $4n+2$

elettroni pi (n numero intero positivo)- regola di Huckel



L'energia di risonanza è la differenza tra l'energia di un ibrido di risonanza e la più stabile delle strutture ipotetiche che a esso contribuiscono.

Una maniera per stimare l'energia di risonanza del benzene è paragonare i calori di idrogenazione del cicloesene e del benzene.

La riduzione catalitica di un alchene è una reazione esotermica.

Il benzene può subire idrogenazione in condizioni estreme.

Idrocarburi policiclici aromatici

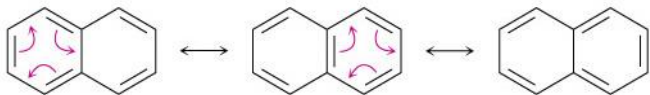
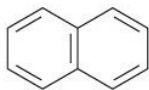
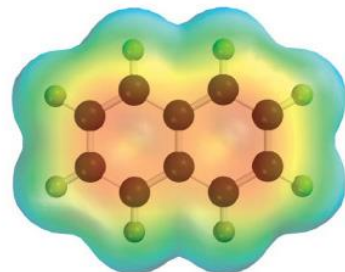
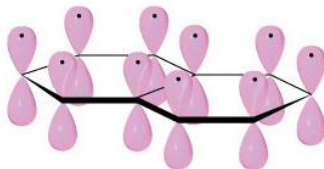


FIGURA 15.12 Il disegno degli orbitali e la mappa di potenziale elettrostatico del naftalene mostrano che i dieci elettroni π sono completamente delocalizzati su entrambi gli anelli.



Naftalene



Requisiti per l'aromaticità:

Molecola ciclica

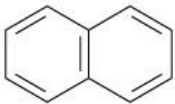
Planare

atomi ibridizzati sp^2

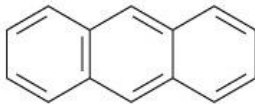
Sistema coniugato continuo di elettroni contenete $4n+2$

elettroni π (n numero intero positivo)- regola di Huckel

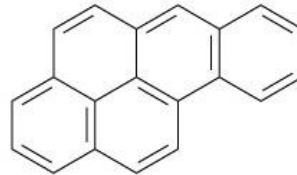
Idrocarburi policiclici aromatici



Naftalene

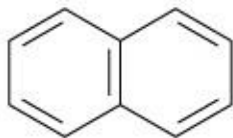


Antracene

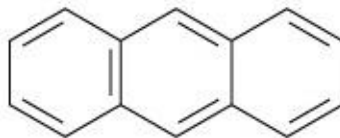


Benzo[a]pirene

3,4-benzopirene



Naftalene



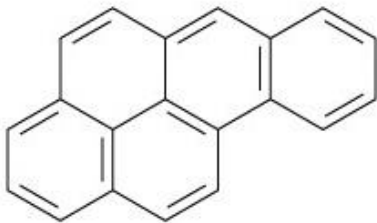
Antracene

Naftalene:

Ottenuto per distillazione del catrame o del carbone.

Antracene:

utilizzato nell'industria dei coloranti e come conservante nell'industria del legname, grazie alle sue proprietà insetticide. Non cancerogeno ma persistente, bioaccumulabile e tossico per gli organismi acquatici



Benzo[a]pirene

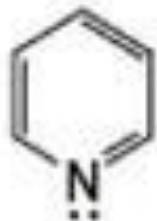
Benzopireni:

contenuti nel catrame, e negli scarti di combustione di molecole ad alto MW. Si formano nella cottura dei cibi alla griglia.

Contenuti nel fumo di sigaretta e negli scarichi dei motori Diesel.

Cancerogeni.

Alcuni eterocicli aromatici



piridina



pirrolo

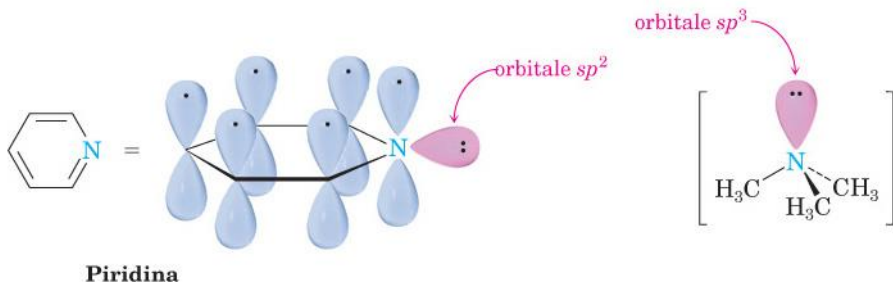


furano



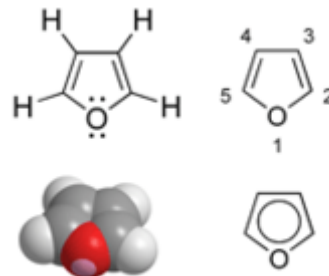
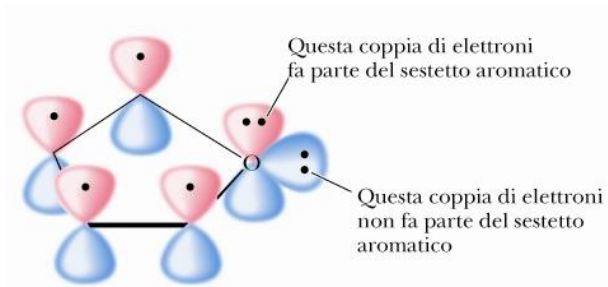
tiofene

Piridina: eterociclo aromatici a sei termini



Il doppietto spaiato dell'azoto non partecipa all'aromaticità: reattività basica

Aromaticità del furano



Requisiti per l'aromaticità:

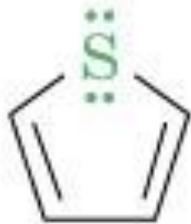
Molecola ciclica

Planare

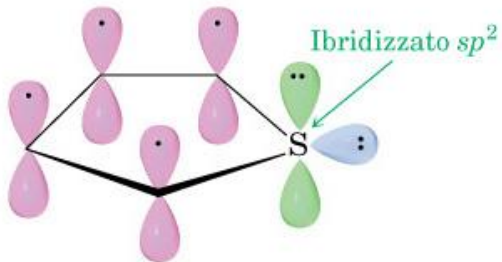
atomi ibridizzati sp^2

Sistema coniugato continuo di elettroni contenete $4n+2$

elettroni π (n numero intero positivo)- regola di Huckel

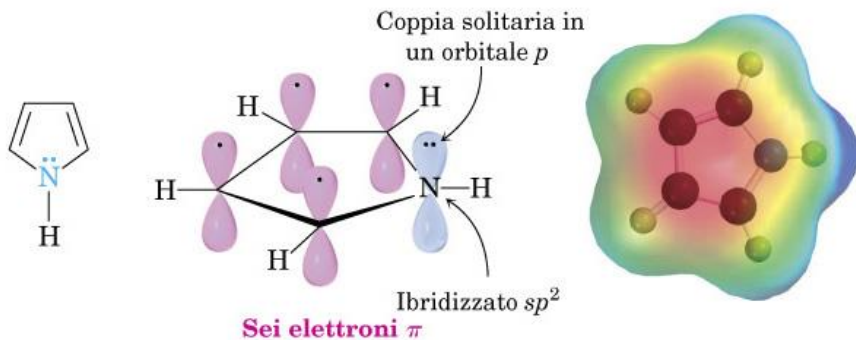


Aromaticità del tiofene



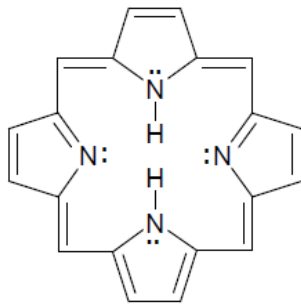
Tiofene

Aromaticità del pirrolo

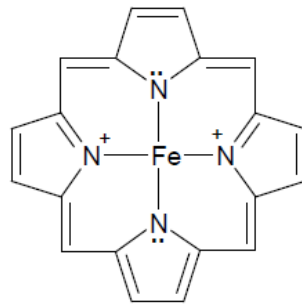


Il doppietto spaiato dell'azoto partecipa all'aromaticità: non ha reattività basica

Il pirrolo gioca un ruolo fondamentale nei sistemi biologici che sono in grado di chelare metalli quali le porfirine:



anello porfirinico



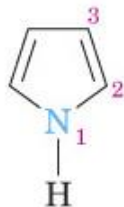
gruppo eme

il sistema a base di queste strutture è la porfina, un sistema coniugato planare a 18 elettroni

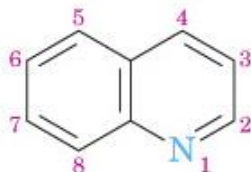
Eterocicli aromatici contenenti N



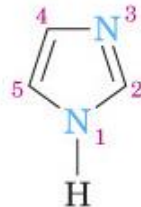
Piridina



Pirrolo



Chinolina



Imidazolo

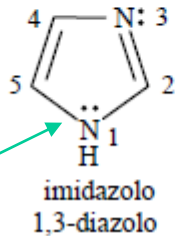


Indolo

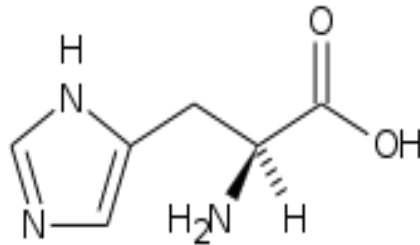
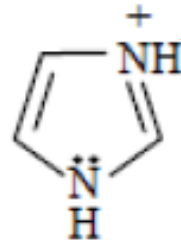


Pirimidina

L'imidazolo

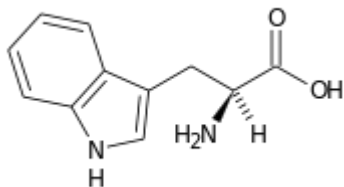
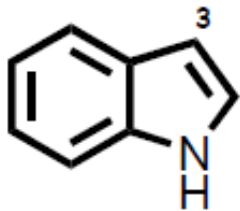


Doppio che
partecipa
all'aromaticità:
no basico

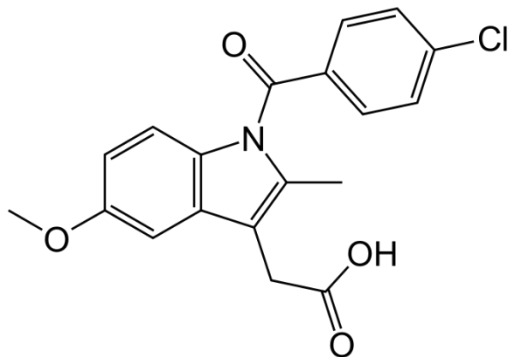


Istidina: un
amminoacido

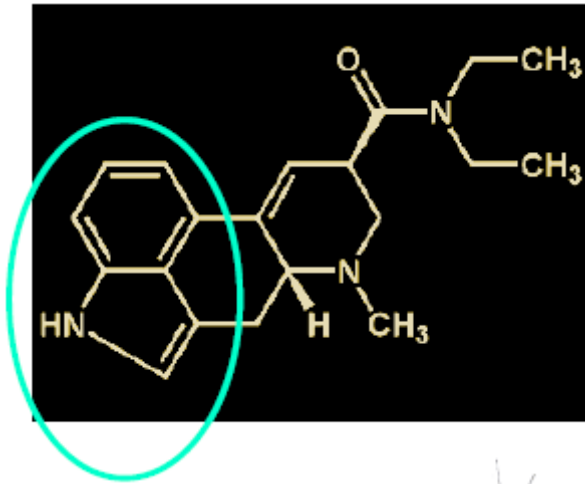
L'indolo



Triptofano (amminoacido)



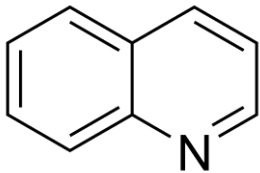
Indometacina
(antiinfiammatorio non steroideo)



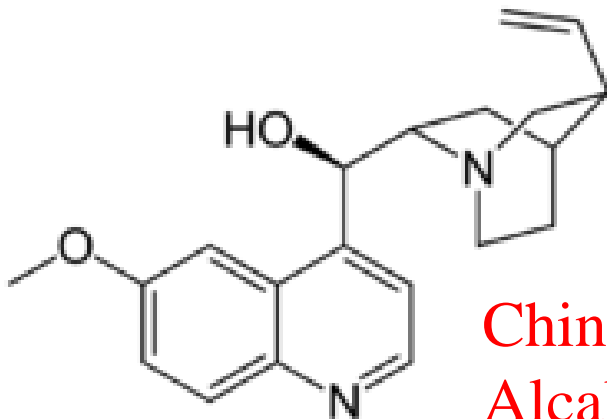
LSD
dietilammide
dell'acido lisergico

Claviceps purpurea è un **ascomicete parassita** delle graminacee il cui nome comune è **ergot**. Genera nelle piante infette degli sclerozi a forma di corna o speroni. Questi sono i corpi fruttiferi del fungo in cui sono contenuti diversi alcaloidi tra cui l'**acido lisergico**. Questi hanno vari tipi di effetti su persone e animali che li assumono. Sono vasocostrittori e **interagiscono con il sistema nervoso centrale** in particolare con i recettori della serotonina.





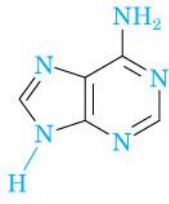
chinolina



Chinino

Alcaloide antimalarico

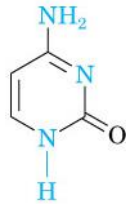
Basi azotate degli acidi nucleici



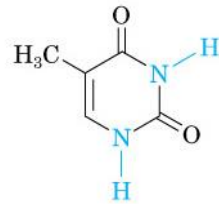
Adenina (A)
DNA
RNA



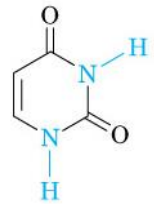
Guanina (G)
DNA
RNA



Citosina (C)
DNA
RNA



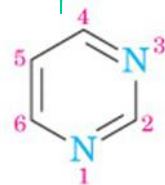
Timina (T)
DNA



Uracile (U)
RNA



Purina

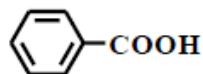


Pirimidina

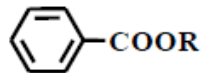


Derivati del benzene

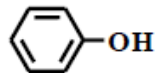
Priorità	Composto base	Nome base	Priorità	Composto base	Nome base
----------	---------------	-----------	----------	---------------	-----------



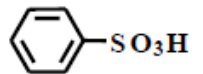
acido benzoico



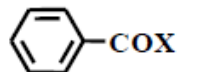
alchil benzoato



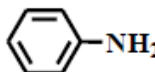
fenolo



acido benzen
solfonico

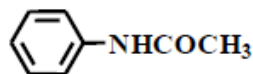


benzoil
alogenuro

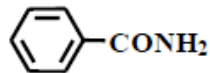


anilina

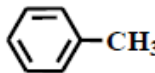
X = Cl, Br



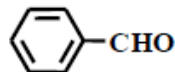
acetanilide



benzammide



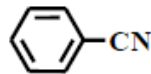
toluene



benzaldeide

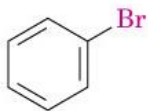


benzene

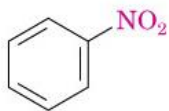


benzonitrile

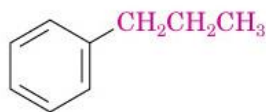
Ulteriori derivati del benzene



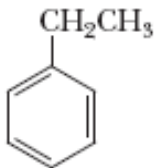
Bromobenzene



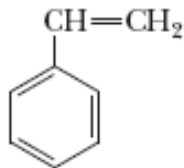
Nitrobenzene



Propilbenzene

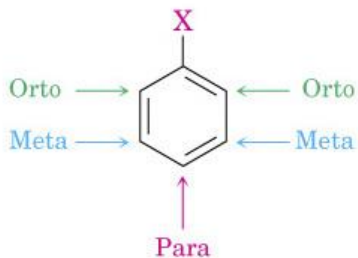


Etilbenzene

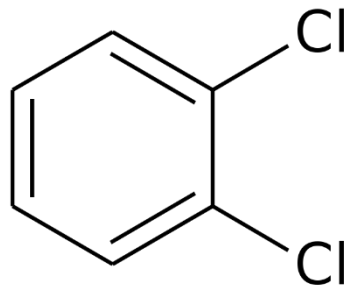


Stirene

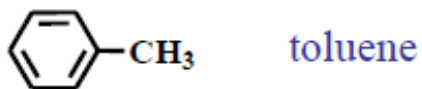
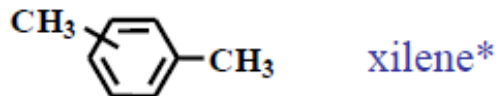
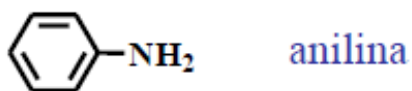
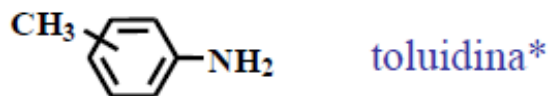
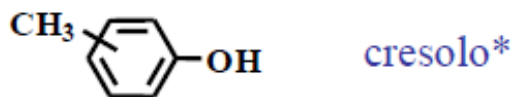
Benzene disostituito



1,2-diclorobenzene
oppure
o-diclorobenzene



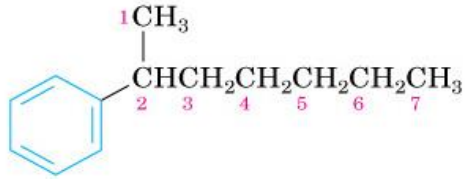
Composto base	Nome base
---------------	-----------



Il gruppo sostituyente fenilico

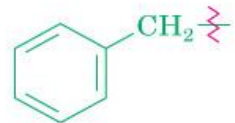


Gruppo fenilico



2-Fenileptano

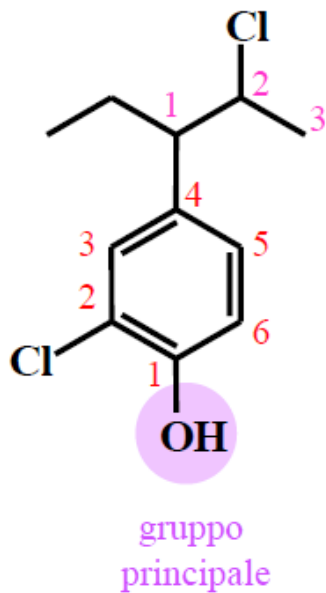
Il gruppo benzilico



Gruppo benzilico

Nomenclatura dei derivati del benzene

Esempio



Numerare gli altri carboni nella direzione che permetta il più basso set di numeri
A parità di numeri, vince il sostituito con iniziale più bassa nell'ordine alfabetico

1. Gruppo principale: **OH**

Fenolo

2. Numerazione anello:

3. Sostituito complesso:

(2-cloro-1-etilpropil)

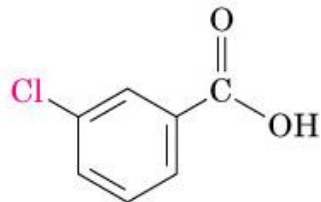
4. Assemblaggio:

2-cloro-4-(2-cloro-1-etilpropil)fenolo

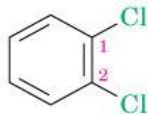
Esempi di nomenclatura dei derivati del benzene



2,6-Dibromofenolo



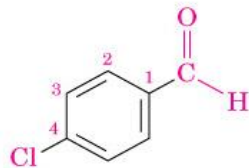
Acido *m*-clorobenzoico



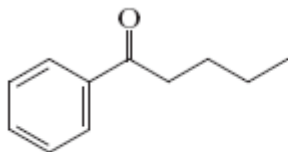
orto-Diclorobenzene
1,2 disostituito



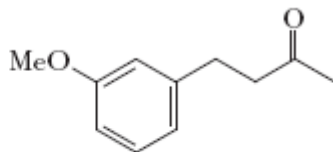
meta-Xilene
1,3 disostituito



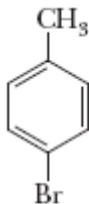
para-Clorobenzaldeide
1,4 disostituito



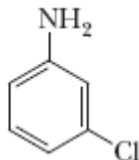
1-Fenil-1-pentanone



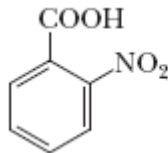
4-(3-Metossifenil)-2-butanone



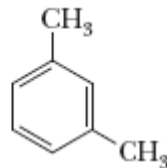
4-Bromotoluene
(*p*-Bromotoluene)



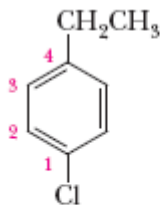
3-Cloroanilina
(*m*-Cloroanilina)



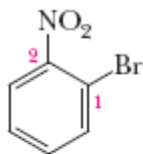
Acido 2-nitrobenzoico
(Acido *o*-nitrobenzoico)



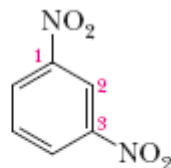
m-Xilene



1-Cloro-4-etilbenzene
(*p*-Cloroetilbenzene)



1-Bromo-2-nitrobenzene
(*o*-Bromonitrobenzene)



1,3-Dinitrobenzene
(*m*-Dinitrobenzene)