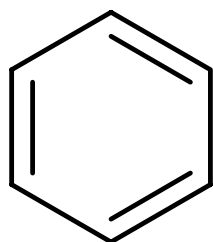


Composti Aromatici: Benzene



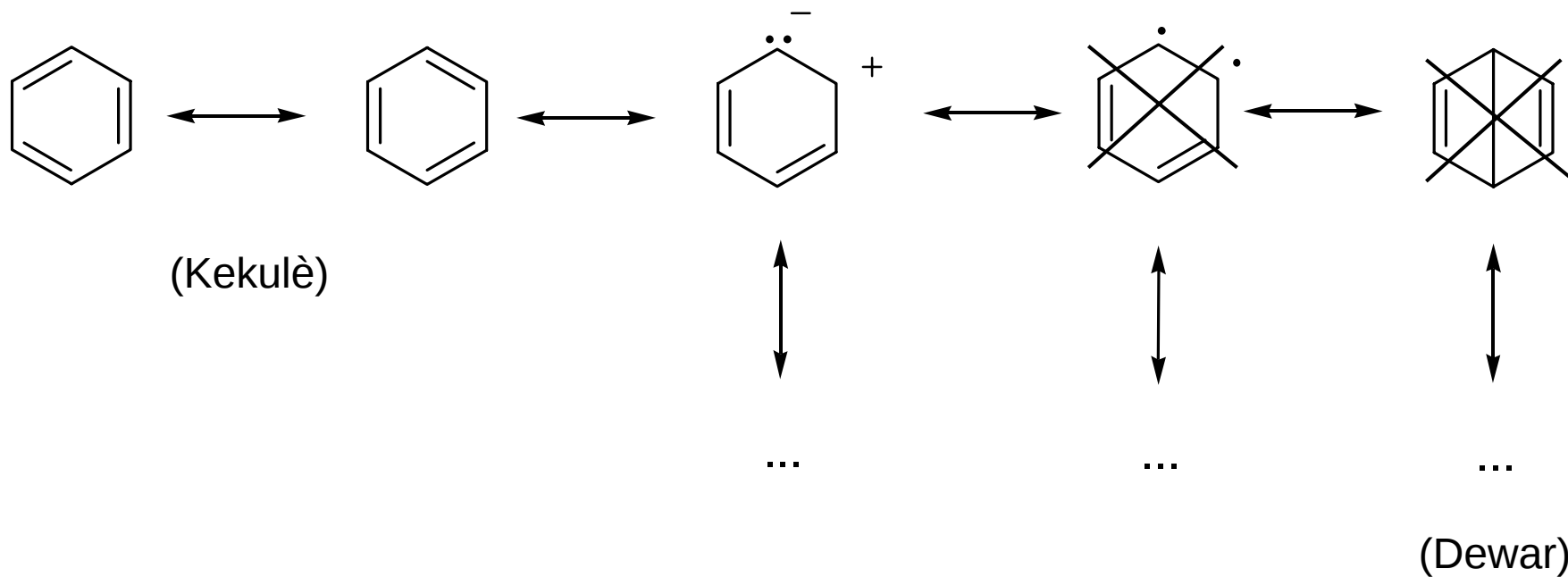
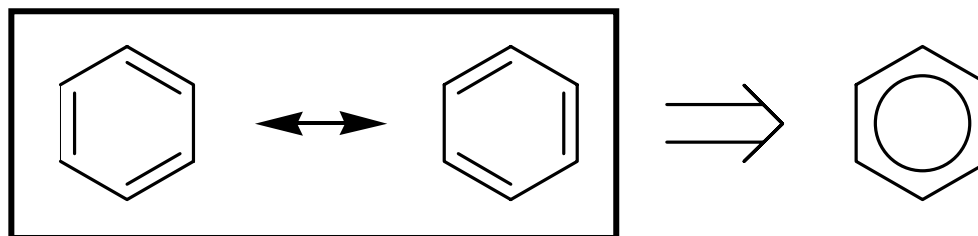
(1865)



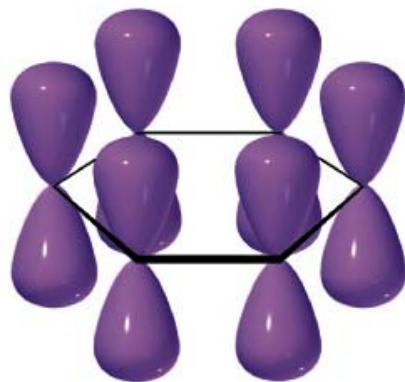
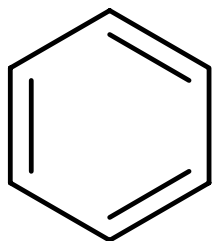
Friedrich August Kekulé

La reattività del benzene è differente dalla reattività tipica delle olefine, anche se coniugate

Composti Aromatici: formule di risonanza



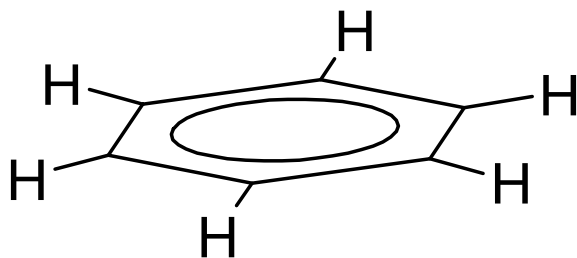
Composti Aromatici: Benzene, orbitali molecolari



6 orbitali atomici p



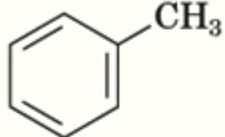
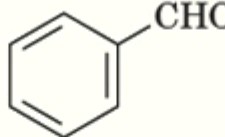
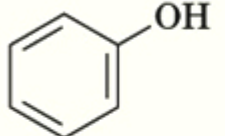
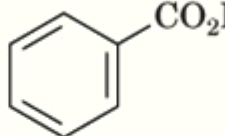
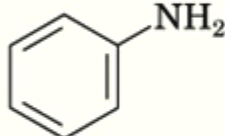
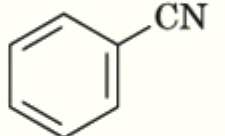
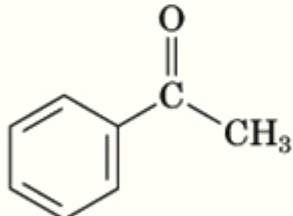
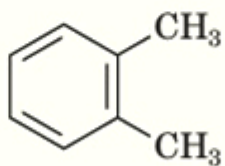
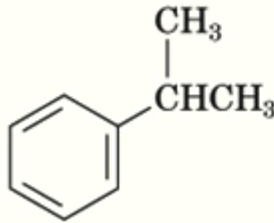
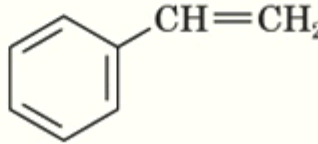
Orbitale π a più
bassa energia



Distanza di legame C-C: 1.40 Å
(C-C: 1.48 Å, C=C: 1.32 Å)

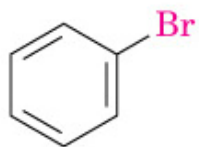
Nomenclatura dei derivati benzene: nomi comuni

TABELLA 15.1 Nomi comuni di alcuni composti aromatici

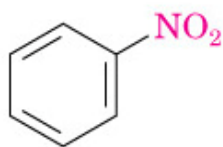
Formula	Nome	Formula	Nome
	Toluene (p.e. 111°C)		Benzaldeide (p.e. 178°C)
	Fenolo (p.f. 43°C)		Acido benzoico (p.f. 122°C)
	Anilina (p.e. 184°C)		Benzonitrile (p.e. 191°C)
	Acetofenone (p.f. 21°C)		<i>orto</i> -Xilene (p.e. 144°C)
	Cumene (p.e. 152°C)		Stirene (p.e. 145°C)

Nomenclatura dei derivati benzene: nomi IUPAC

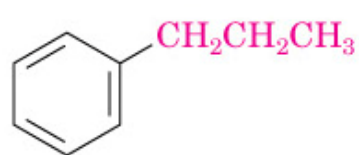
Derivati monosostituiti



Bromobenzene



Nitrobenzene

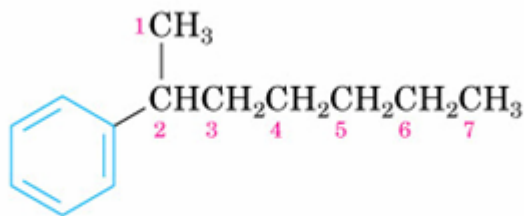


Propilbenzene

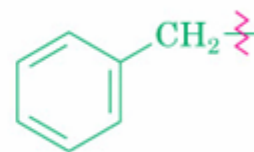
Sostituenti:



Gruppo fenilico



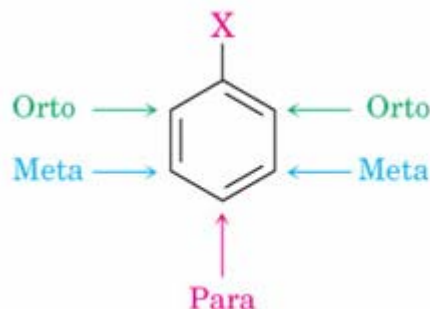
2-Fenileptano



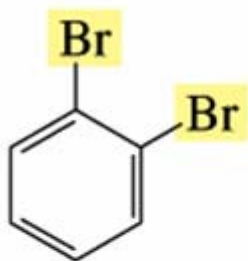
Gruppo benzilico

Nomenclatura dei derivati benzene: nomi IUPAC

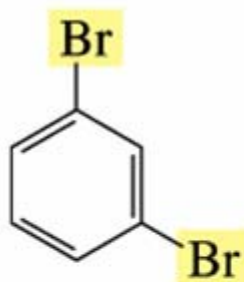
Derivati polisostituiti



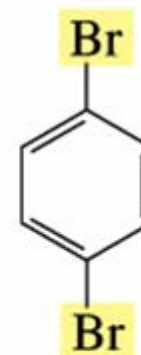
Si numera l'anello in modo che i sostituenti abbiano i numeri più bassi possibili.



1,2-dibromobenzene
***ortho*-dibromobenzene**
***o*-dibromobenzene**



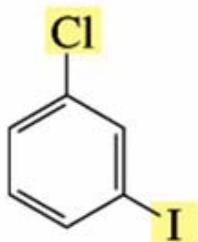
1,3-dibromobenzene
***meta*-dibromobenzene**
***m*-dibromobenzene**



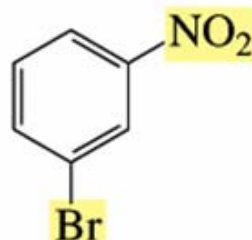
1,4-dibromobenzene
***para*-dibromobenzene**
***p*-dibromobenzene**

Nomenclatura dei derivati benzene: nomi IUPAC

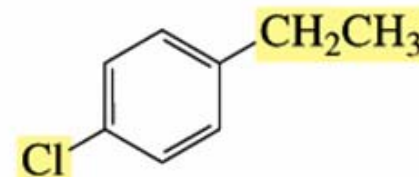
Se ci sono due sostituenti diversi, si usa l'ordine alfabetico



1-chloro-3-iodobenzene
meta-chloriodobenzene
 not
 1-iodo-3-chlorobenzene
meta-iodochlorobenzene

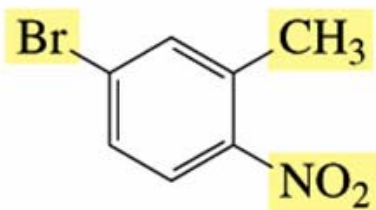


1-bromo-3-nitrobenzene
meta-bromonitrobenzene

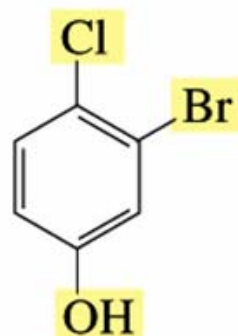


1-chloro-4-ethylbenzene
para-chloroethylbenzene

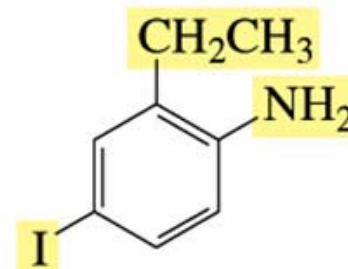
Se si usa un nome comune, il sostituito del composto monofunzionale di cui si usa il nome diventa il sostituito principale.



5-bromo-2-nitrotoluene

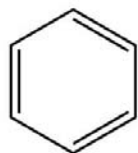
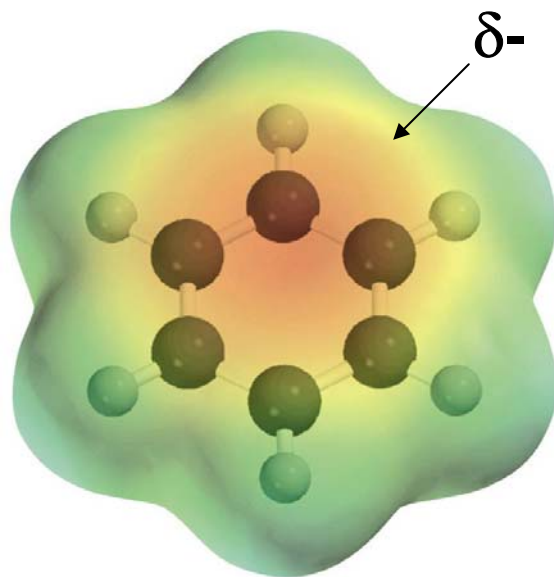


3-bromo-1-chlorophenol

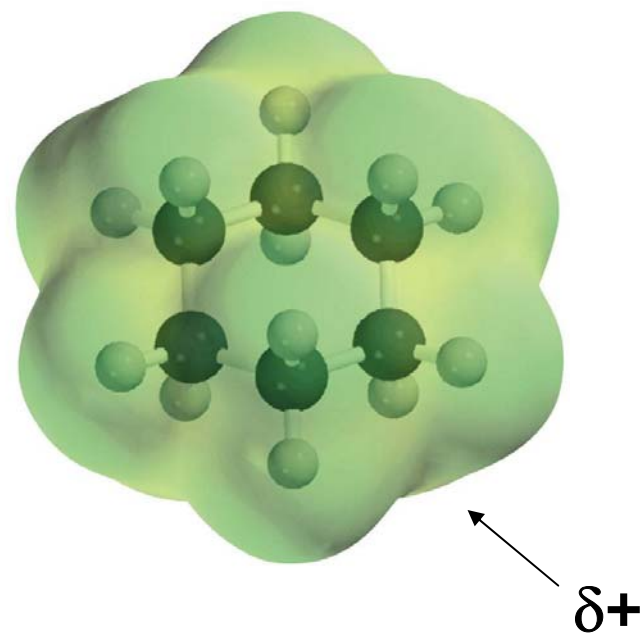


2-ethyl-4-iodoaniline

Reattività del benzene

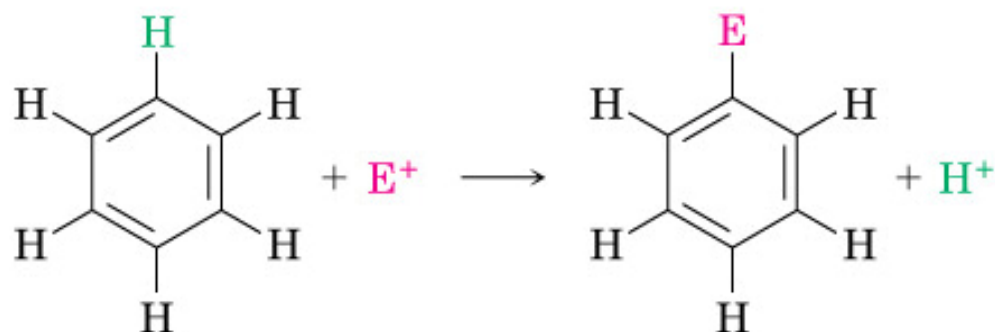
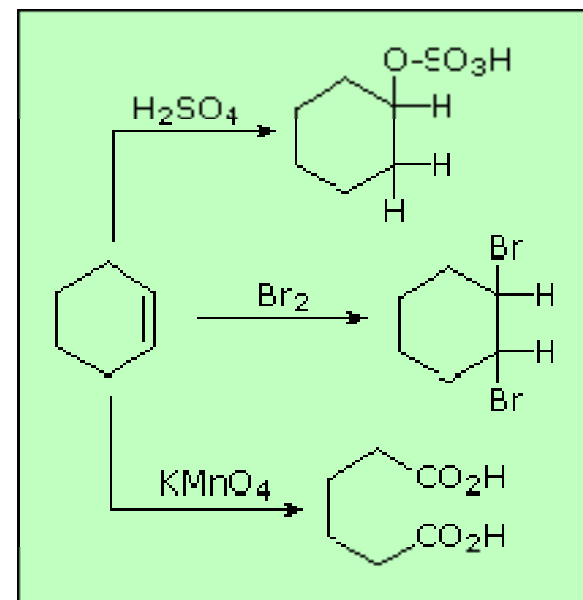
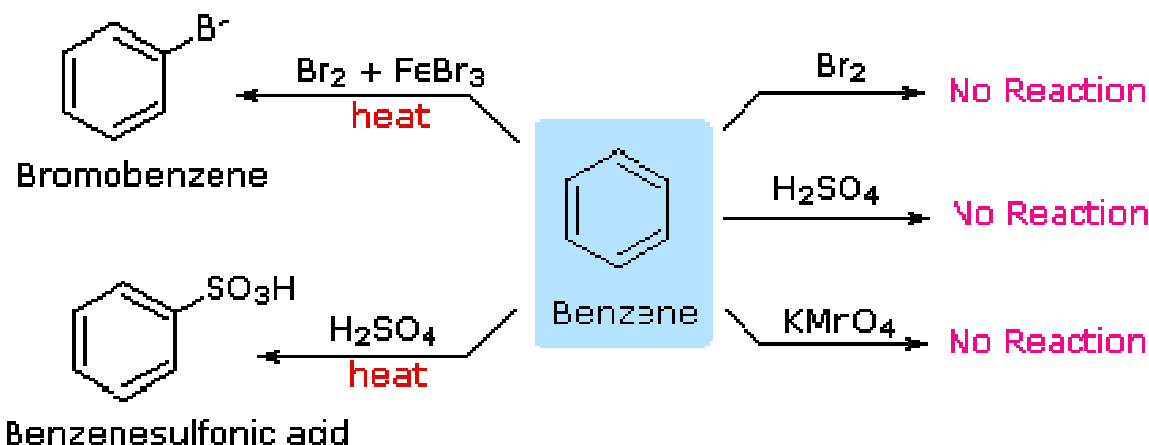


benzene

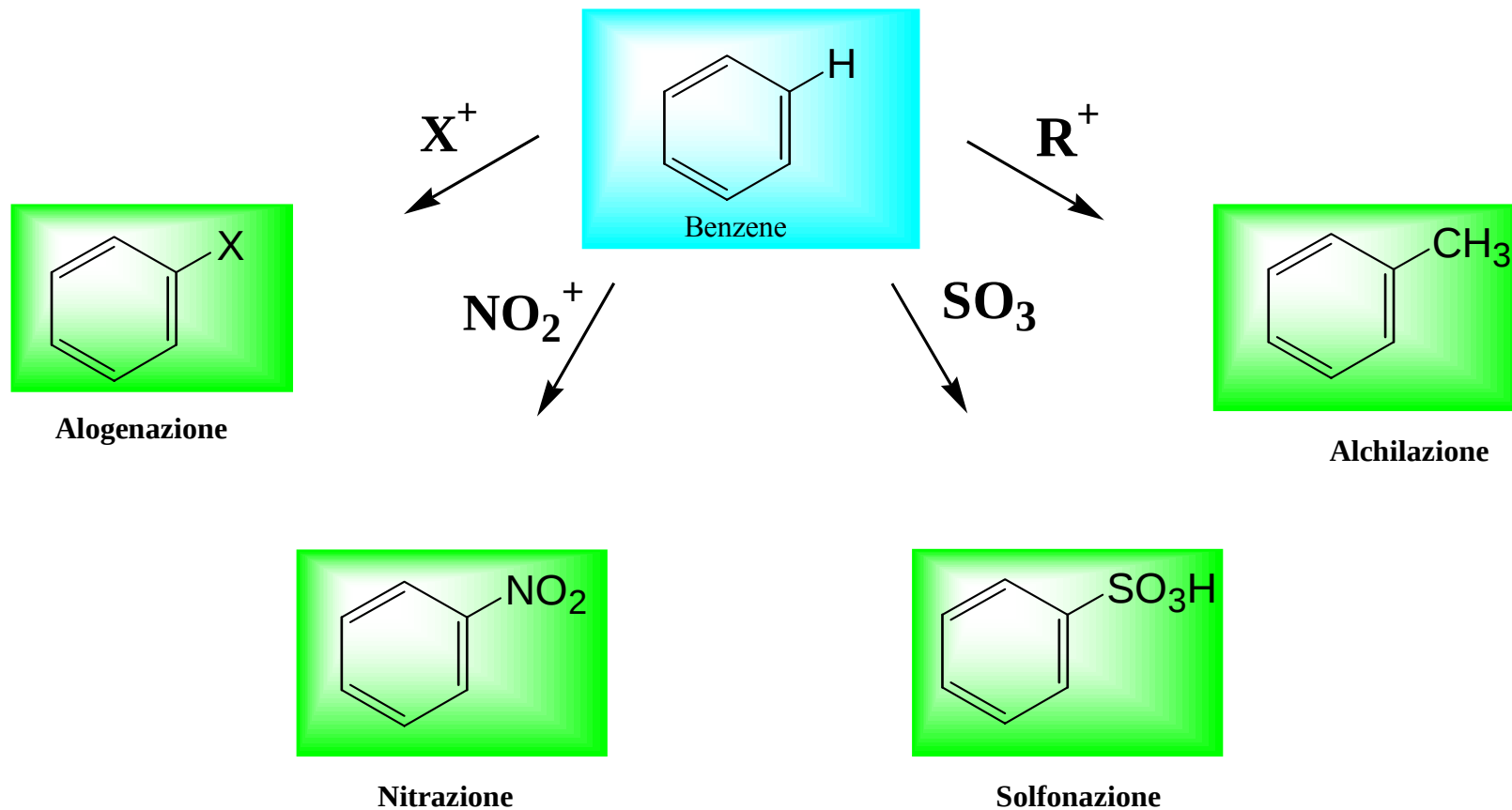


cyclohexane

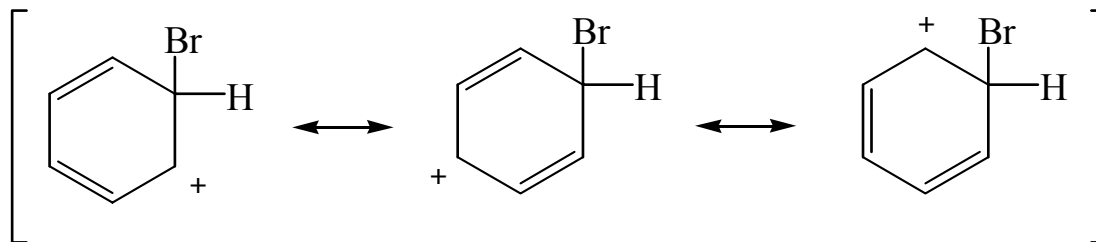
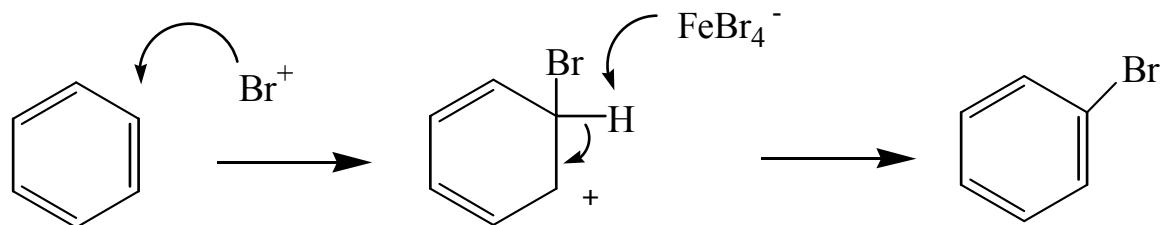
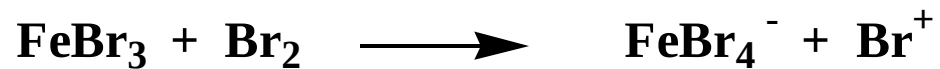
Reattività del benzene: sostituzione



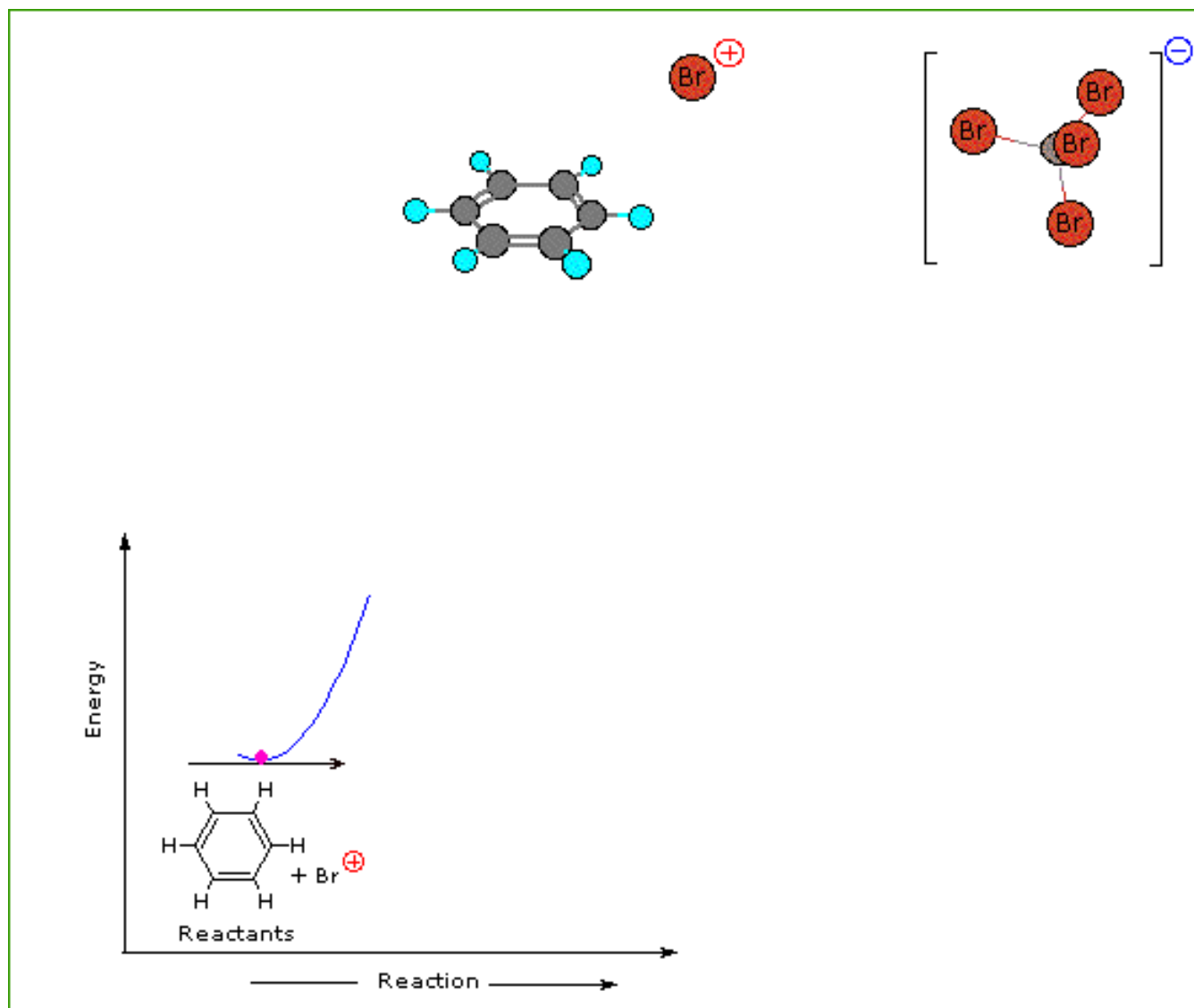
Reattività del benzene: sostituzione



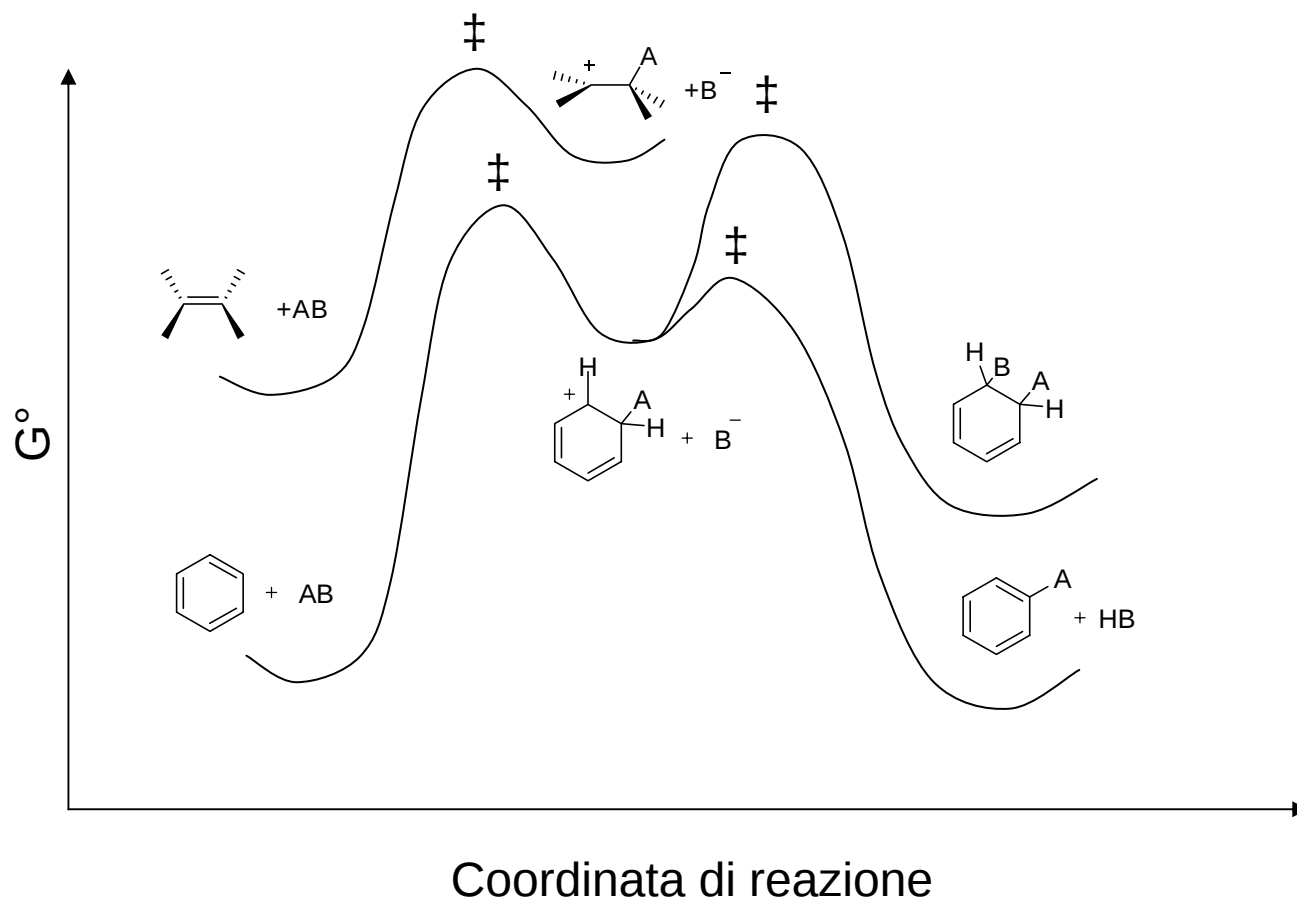
Reattività del benzene



Sostituzione elettrofila aromatica

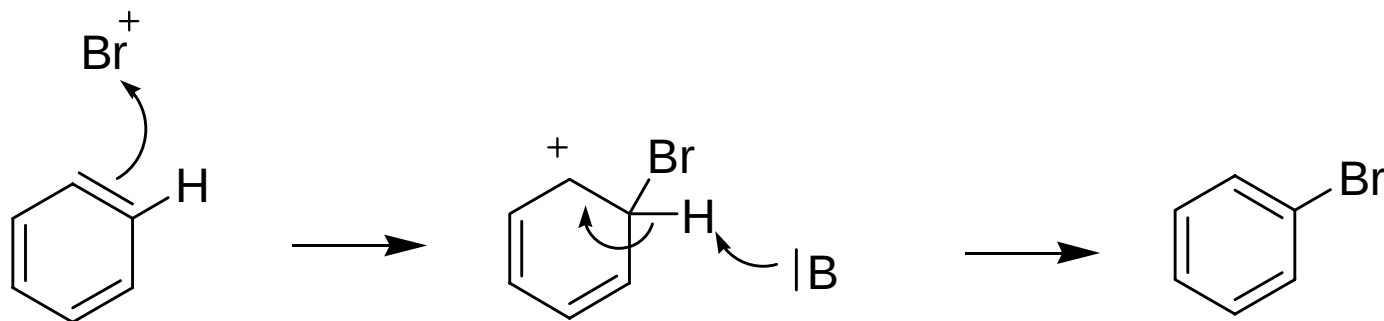
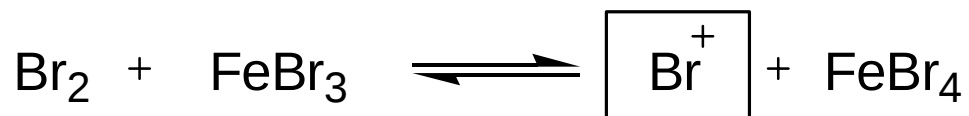


Sostituzione elettrofila vs addizione elettrofila



Sostituzione elettrofila aromatica: reazioni

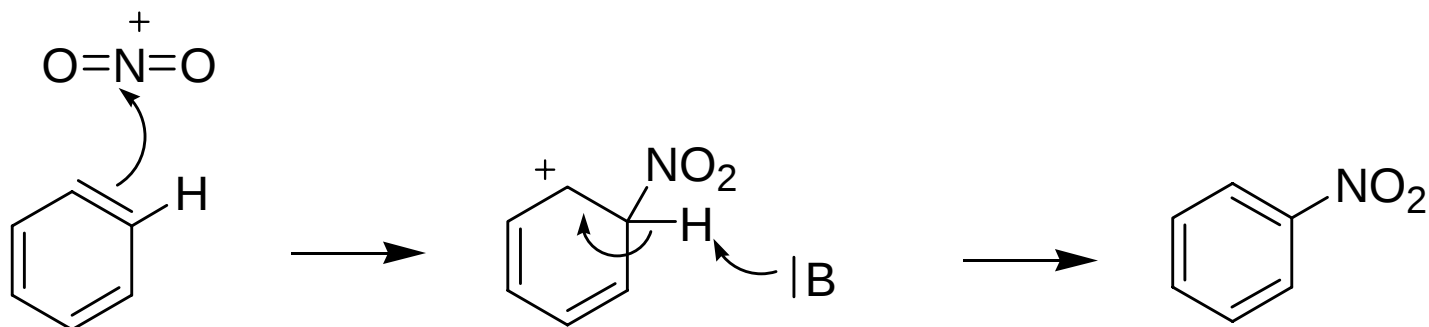
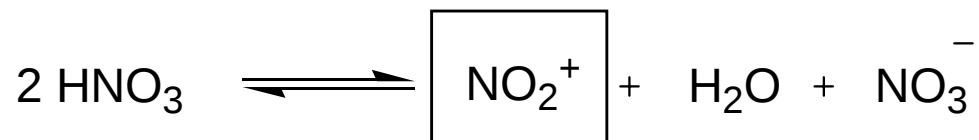
1) Alogenazione



$\text{X} = \text{Cl}, \text{Br}, \text{I}$

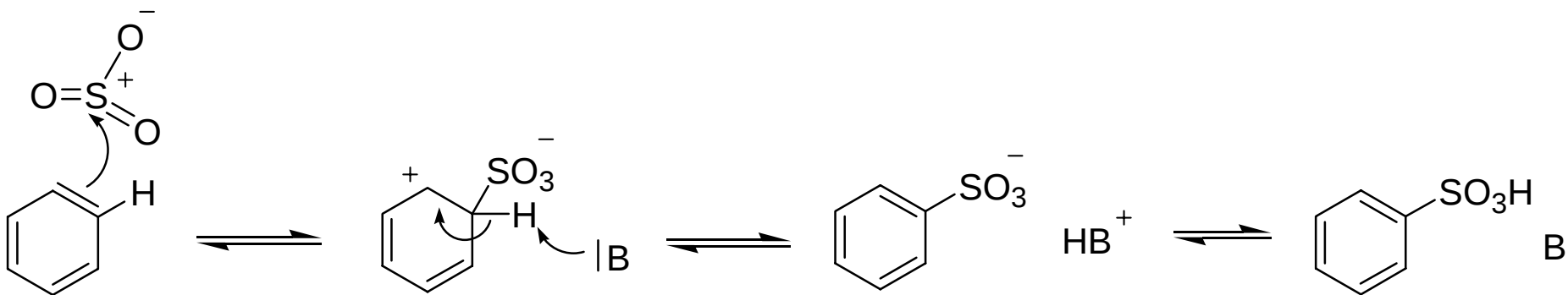
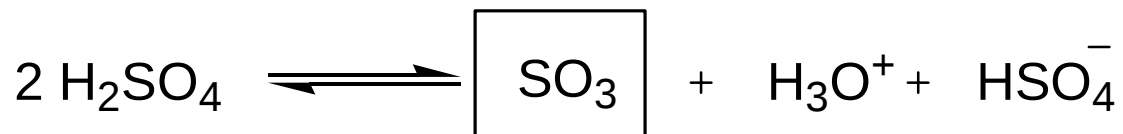
Sostituzione elettrofila aromatica: reazioni

2) Nitrazione



Sostituzione elettrofila aromatica: reazioni

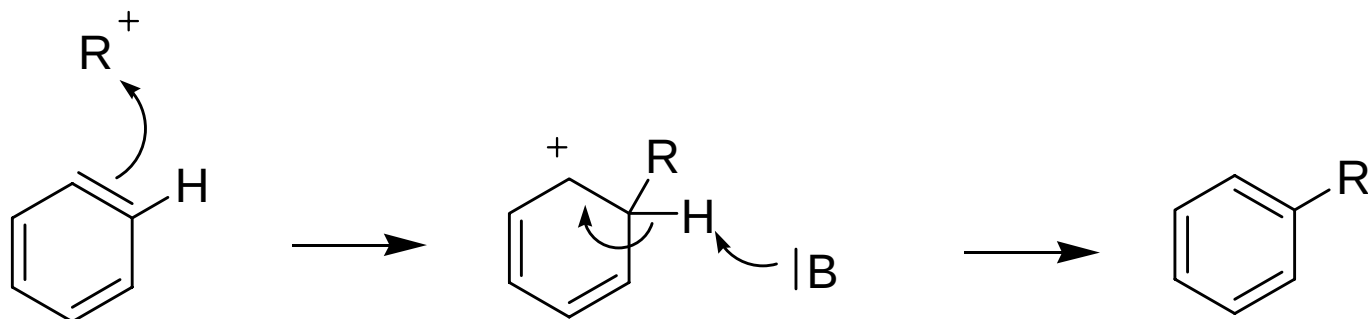
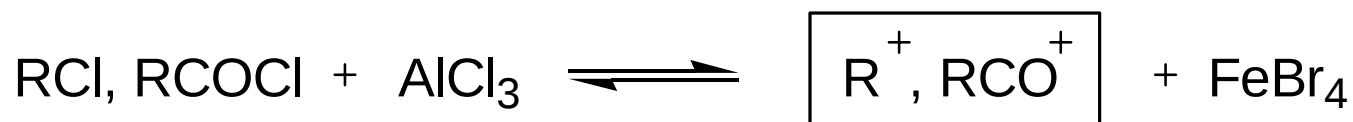
3) Solfonazione



Reazione reversibile!

Sostituzione elettrofila aromatica: reazioni

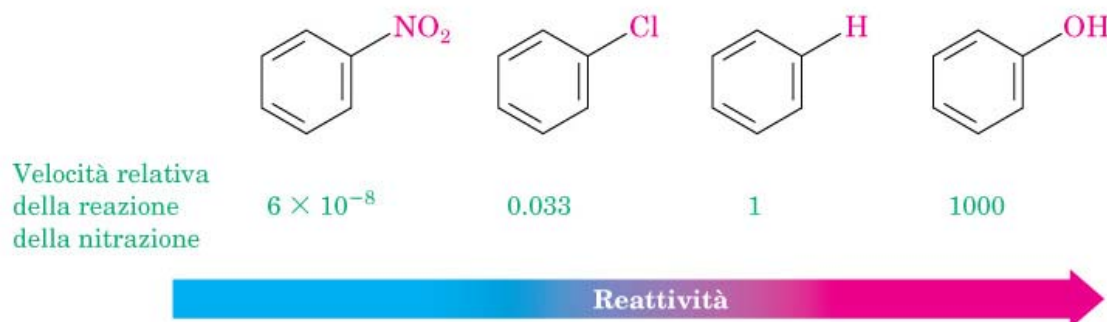
4) Alchilazione/Acilazione di Friedl-Craft



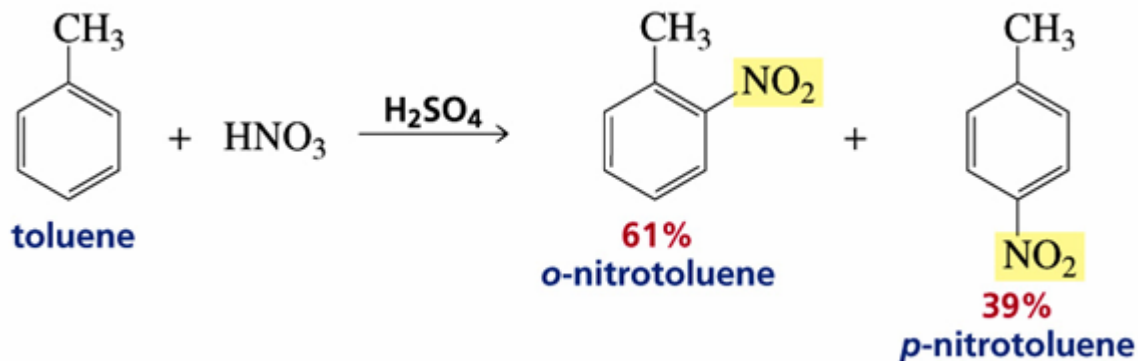
- La reazione non va in sistemi aromatici disattivati
- Solo alogenuri alchilici
- Polisostituzione nelle acilazioni

Effetto dei sostituenti

Velocità della reazione



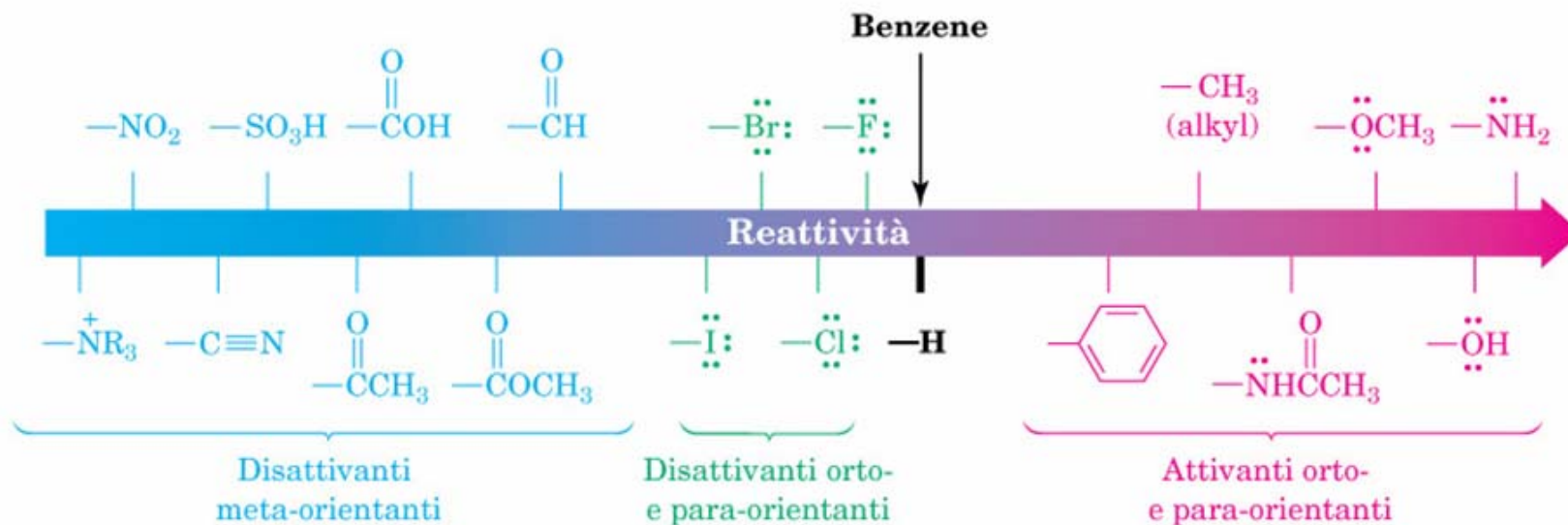
Orientazione



Sostituzione elettrofila aromatica: attivazione e orientazione

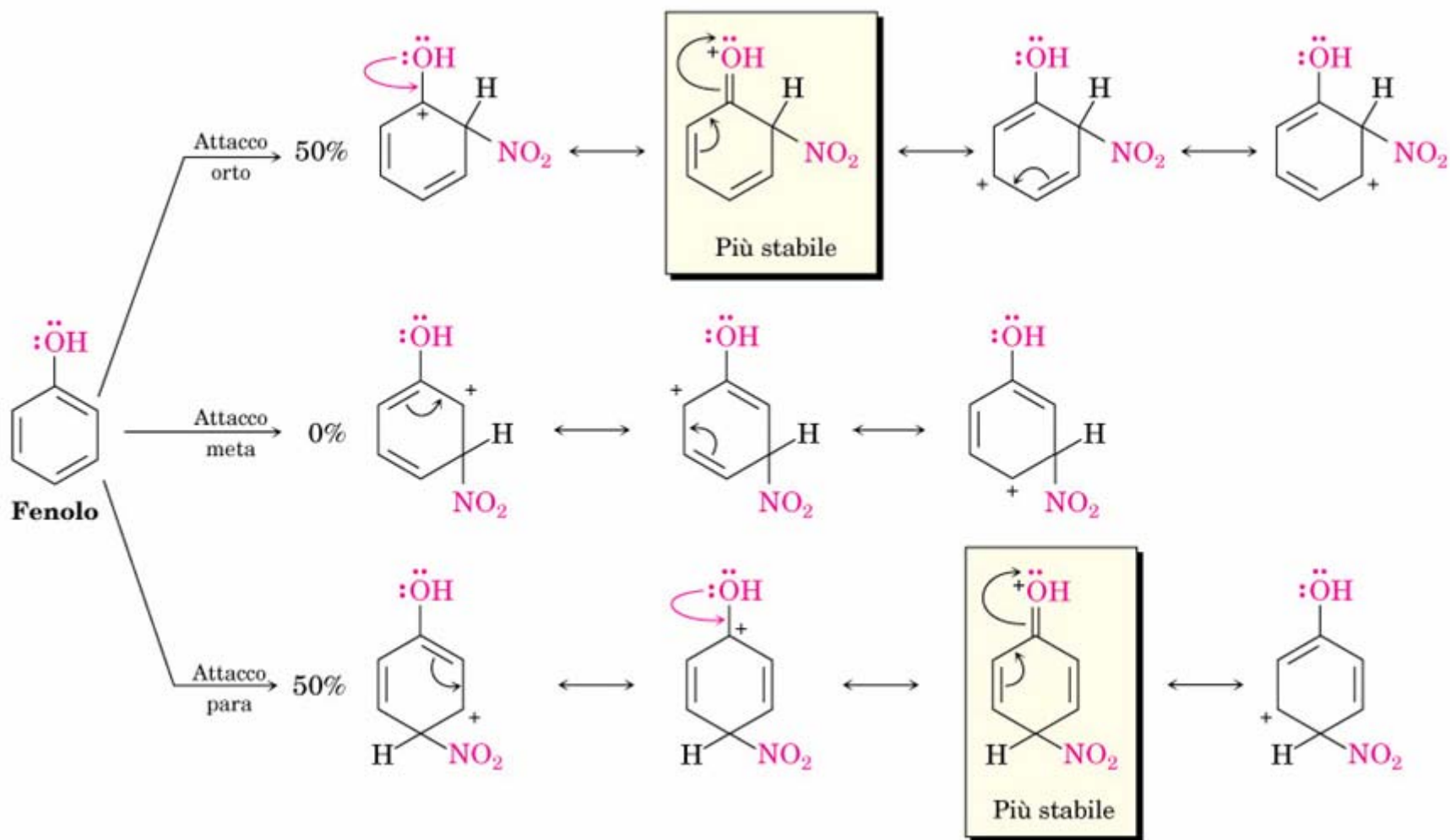
Un gruppo è un **attivante** se è capace di donare elettroni all'anello

Un gruppo è un **disattivante** se sottrae elettroni all'anello

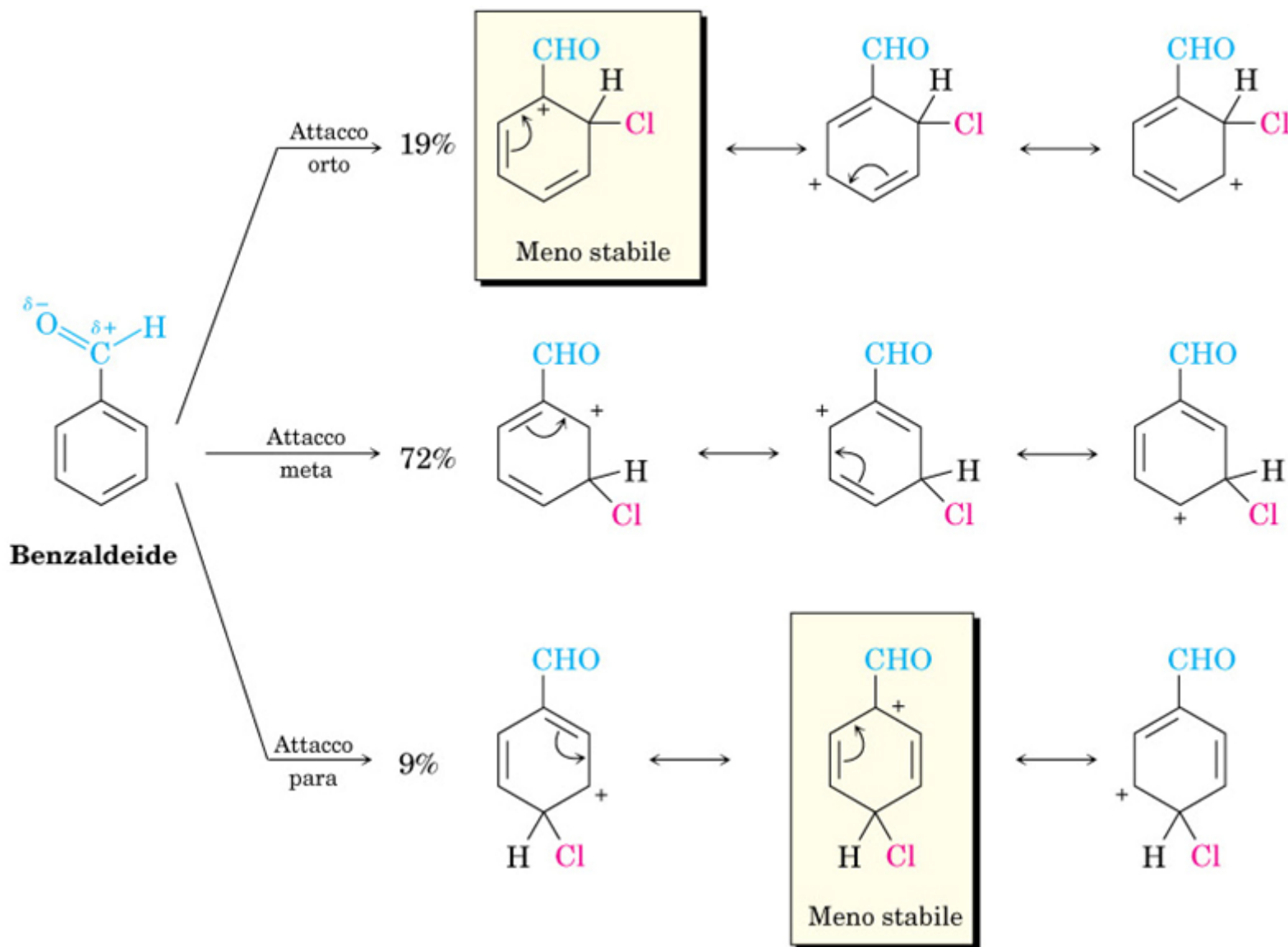


La donazione e l'attrazione degli elettroni possono essere dovuti a un effetto **induttivo** (elettronegatività) o a un effetto di **risonanza** (sovrapposizione tra orbitali p).

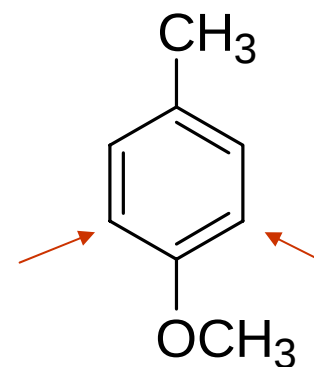
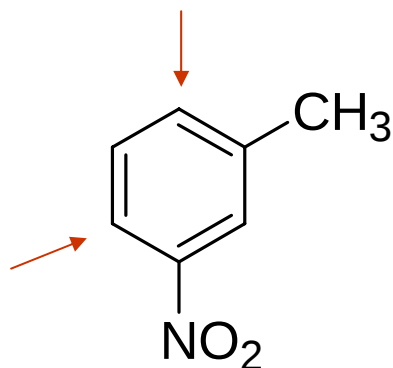
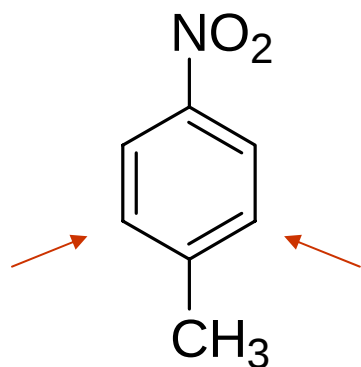
Effetto dei sostituenti: attivanti orto-para orientanti



Effetto dei sostituenti: disattivanti meta-orientati

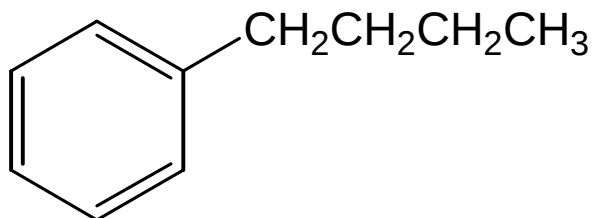


Sostituzione elettrofila aromatica: orientazione

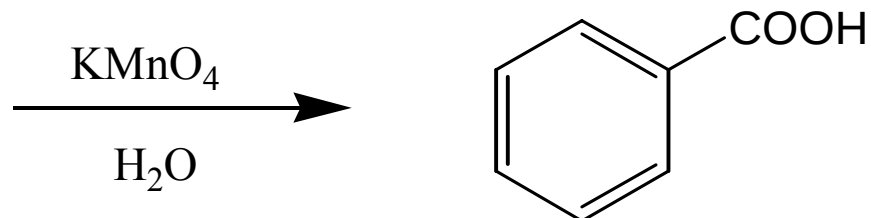


- ✓ Il gruppo attivante prevale sul disattivante.
- ✓ L'attivante forte prevale sull'attivante debole.
- ✓ Bisogna tener conto degli effetti sterici.

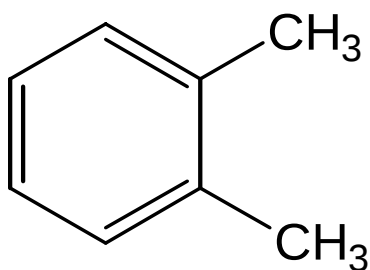
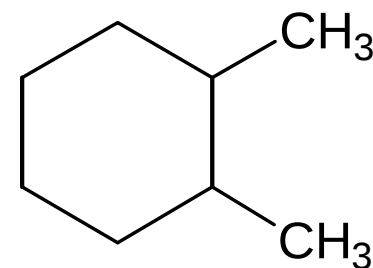
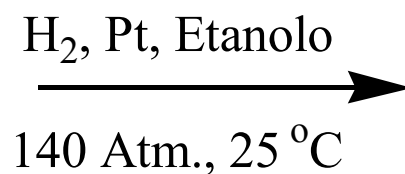
Ossidazione e riduzione dei composti aromatici



Butilbenzene

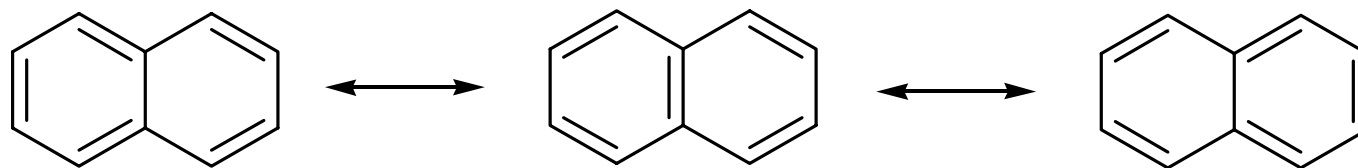


Acido Benzoico

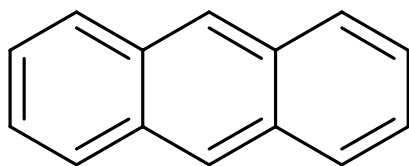
1,2-Dimetilbenzene
o-Xilene

1,2-Dimetilcicloesano

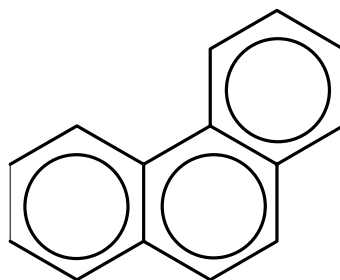
Altri composti aromatici



Naftalene

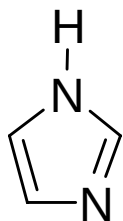
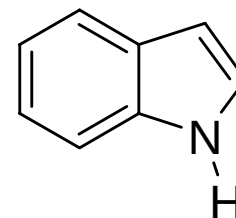
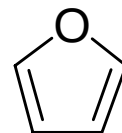
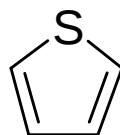
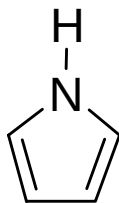
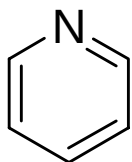


Antracene

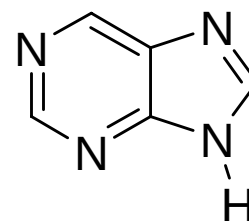
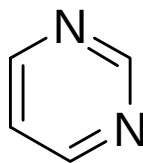


Fenantrene

Composti eteroaromatici



Amminoacidi
(His)



Nucleobasi,
caffeina