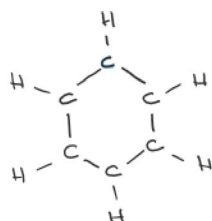
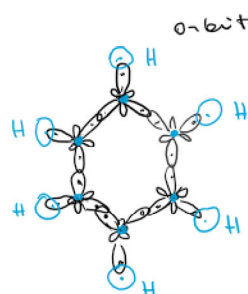


BENZENE

struttura

Tutti i C del benzene sono ibridizzati sp^2

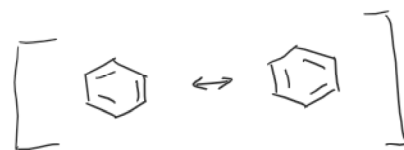


legami σ
ottenuti a partire
dagli orbitali
ibridi sp^2

legami tutti nello
stesso piano



Teoria della risonanza

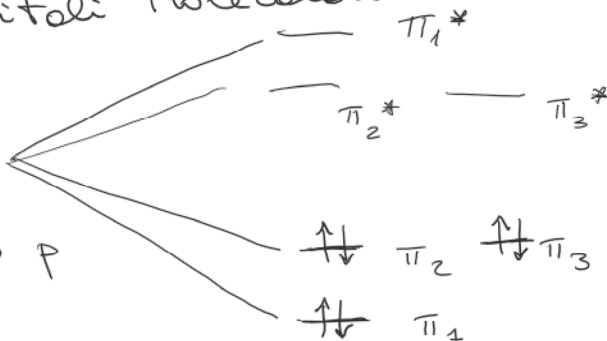


Teoria degli Orbitali Molecolari

E ↑

↑ ↑ ↑ ↑ ↑ ↑

Six orbitali
atomici di tipo p



OM
di
Antilegame

OM
di legame

π_1



π_2



π_3



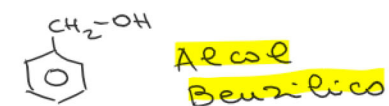
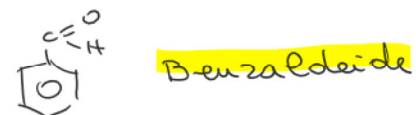
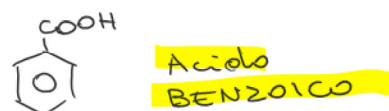
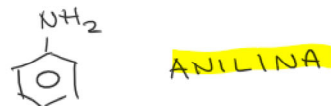
La risonanza che caratterizza il benzene è

- è molto stabile
- ha una reattività particolare

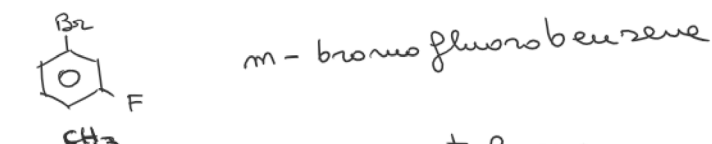
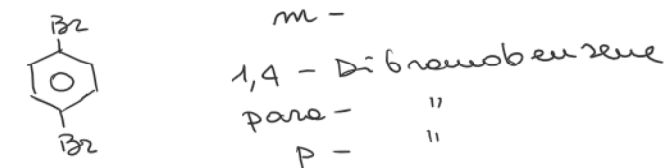
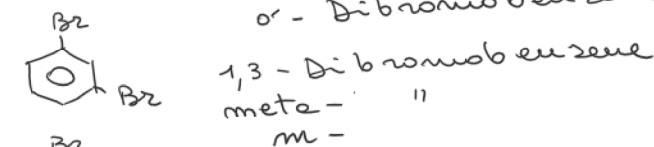
Regole di traccia
Un compito è oromestico se rispetta 3 criteri:

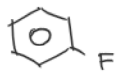
- Deve essere PLANARE
 - Deve essere CICLICO
 - Deve possedere $4n+2$ elettroni π
- Per il benzene con $n=1 \Rightarrow 6$ elettroni π

Benzeni Mono sostituiti:

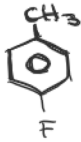


 1,2-Dibromobenzene
 ortho-Dibromobenzene
 o-Dibromobenzene

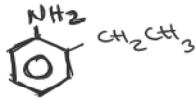




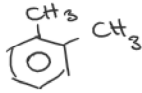
m-bromofluorobenzene



p-fluorotoluene

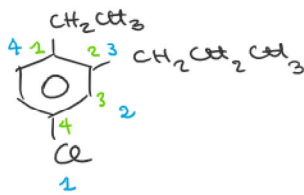


o-ethylamine



o-xylene

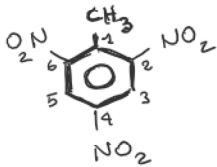
Anelli con più di 2 sostituenti:



1, 2, 4

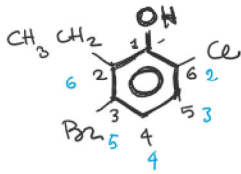
1, 3, 4

4-chloro-1-ethyl-2-propylbenzene



-NO₂ gruppo NITRO

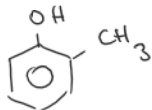
2,4,6-Trinitrotoluene



2, 3, 6

2, 5, 6

3-bromo-6-chloro-2-ethylphenol

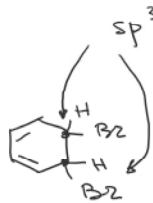


o-cresol

REATTIVITA'

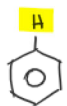


BENZENE
AROMATICO



PRODOTTO
NON AROMATICO

Reazione di Addizione



+ Br₂

FeBr₃



+ HBr

Reazione di Sostituzione

PRODOTTO AROMATICO!

SOSTITUZIONI ELETTROFILE AROMATICHE

1. ALOGENAZIONE (Bromurazione o Clorurazione)

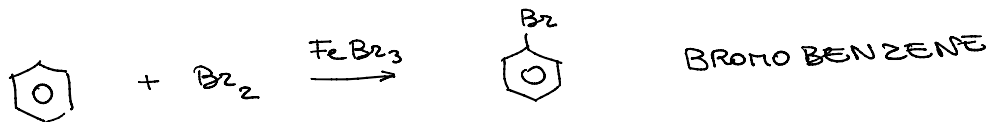
-

FeBr₃

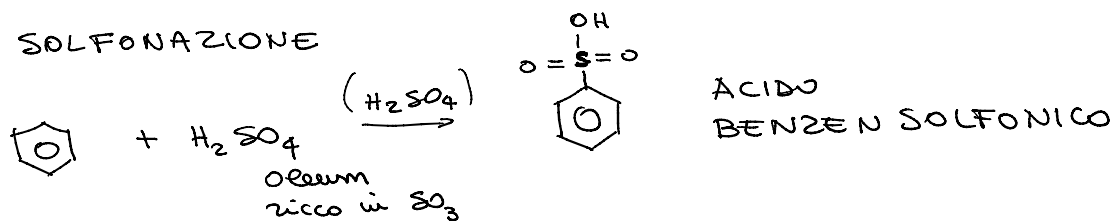


AROMO BENZENE

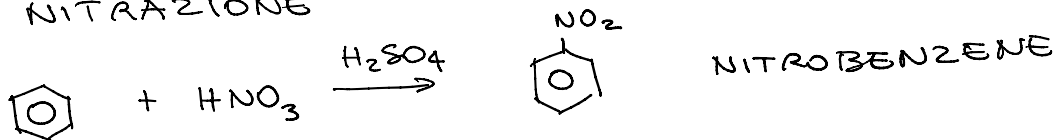
1. ALOGENAZIONE (di un benzene)



2. SOLFONAZIONE

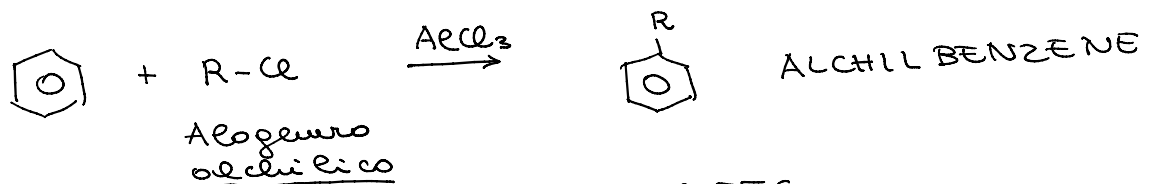


3. NITRAZIONE

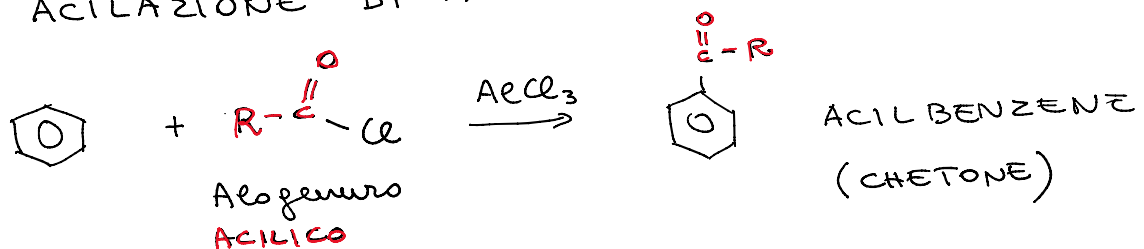


4. ALCHILAZIONE DI FRIEDEL-CRAFTS

↳ entra in anello un gruppo alchilico (metile, etile, isopropile...)

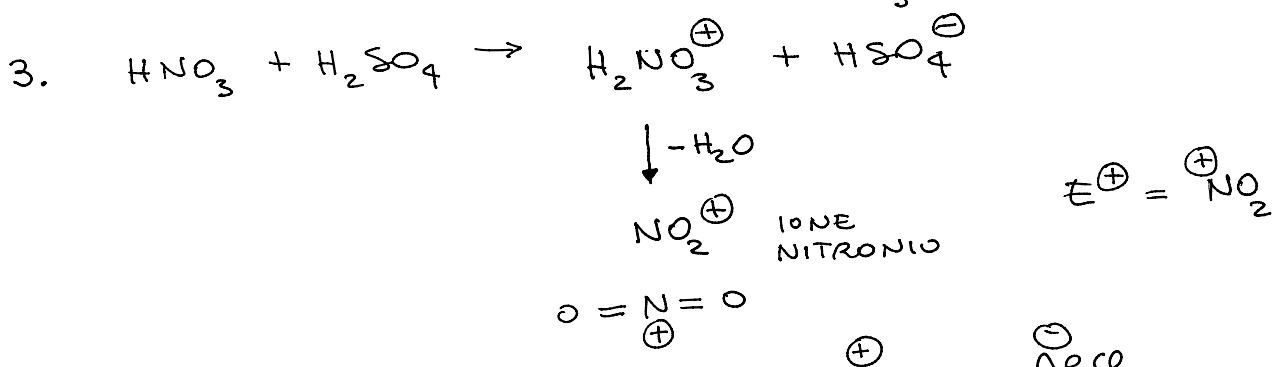
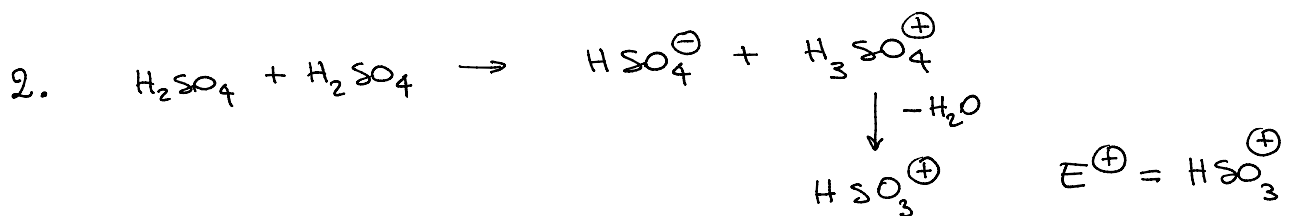


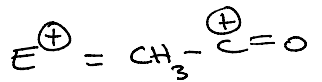
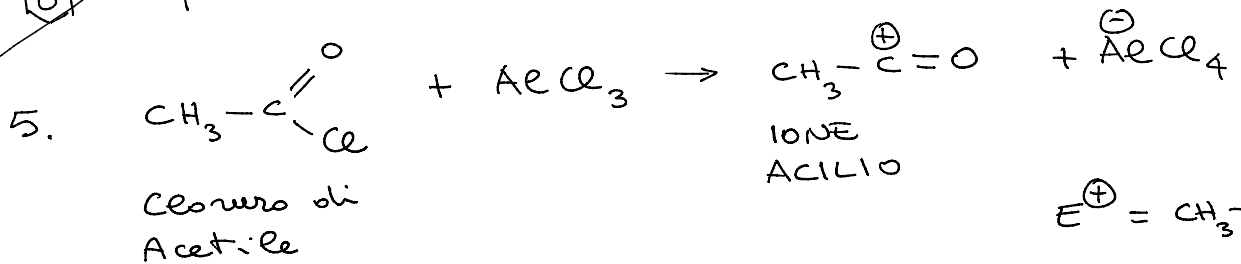
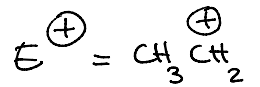
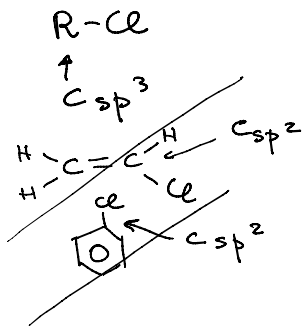
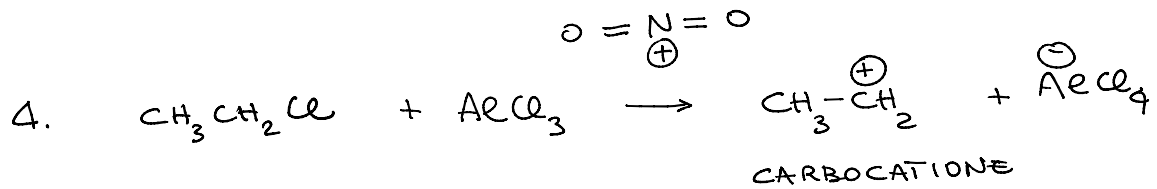
5. ACILAZIONE DI FRIEDEL-CRAFTS



PRESTADIO

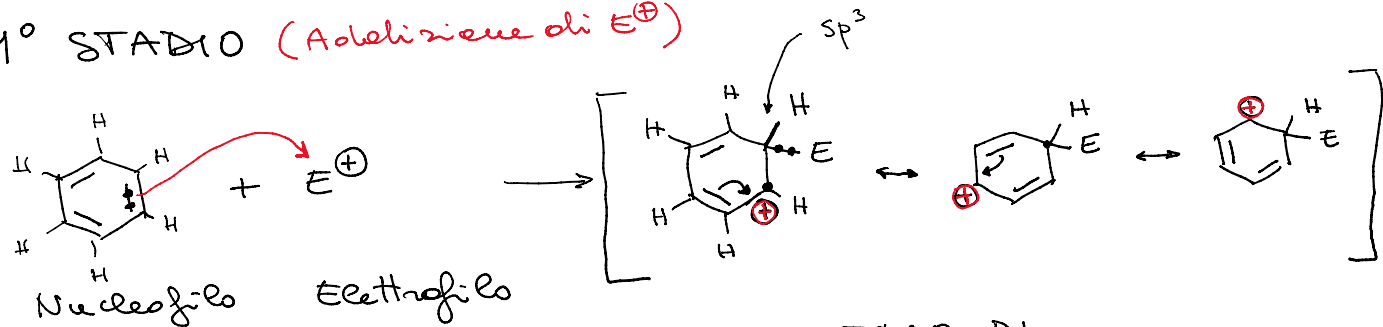
viene prodotto l'elettrofilo grazie al catalizzatore





MECCANISMO DELLA SOSTITUZIONE ELETTROFILA AROMATICA (BISTADIO)

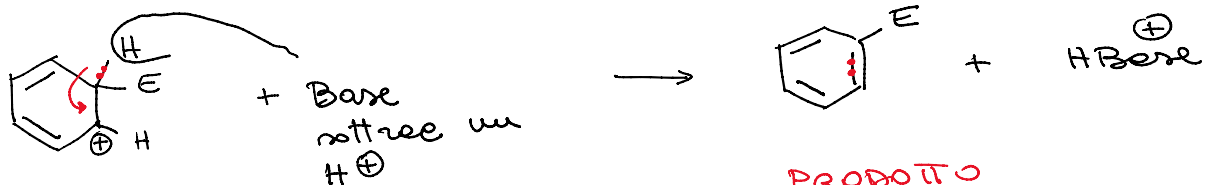
1° STADIO (Addizione di E^+)



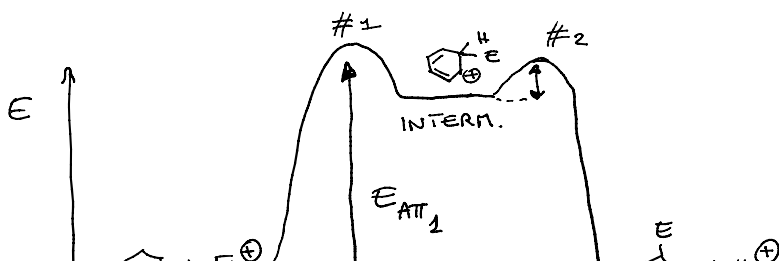
E^+ AROMATICO

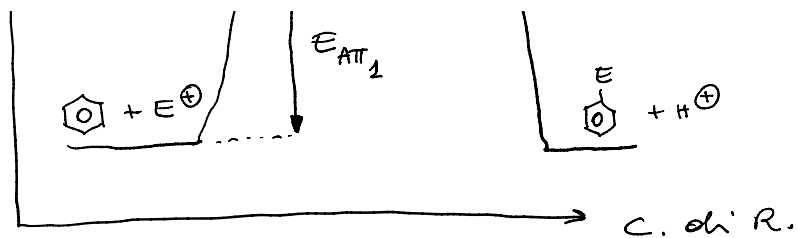
INTERMEDIO DI REAZIONE (WHELAND)
 Stabilizzato per risonanza
 MA NON E' AROMATICO
 (ciclico ma non planare)

2° STADIO (Eliminazione di H^+)



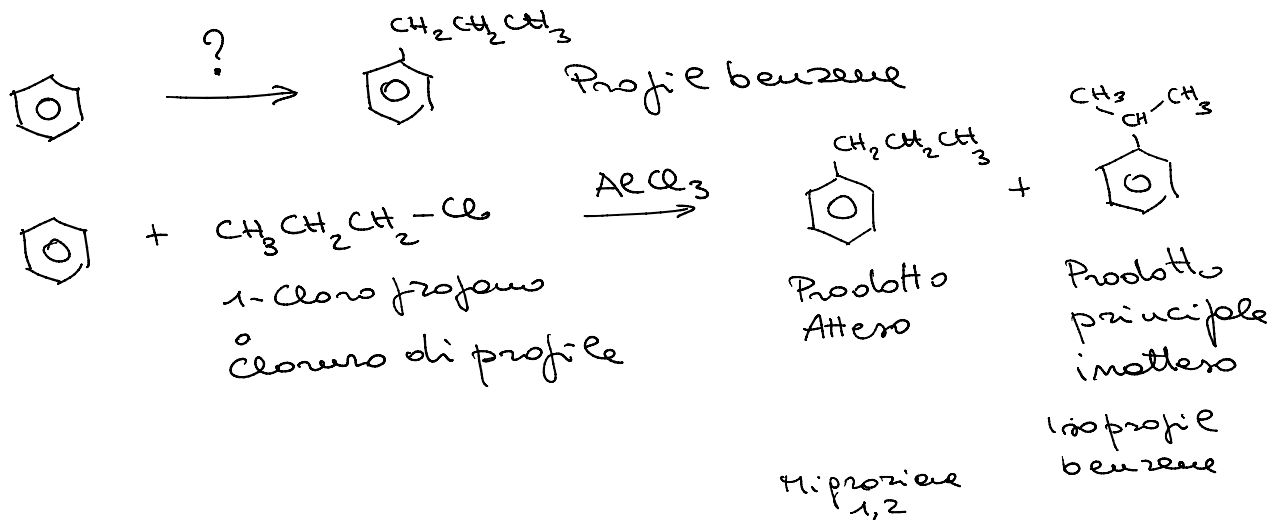
PRODOTTO AROMATICO



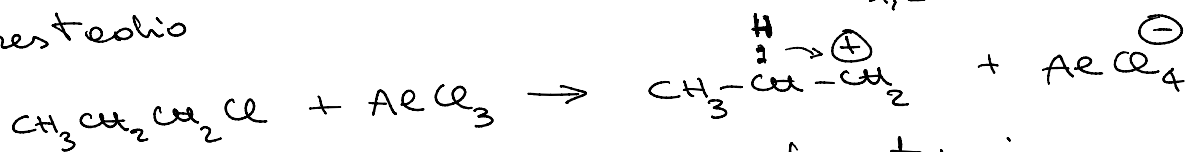


LIMITAZIONI DELL'ACCHILAZIONE DI F.-C.

1.



Pretesto



I carbocationi possono TRASPORRE!

