Chapter 16 - Chemistry of Benzene: Electrophilic Aromatic Substitution

Synthesis Strategies

In order to think about multi-step synthesis, it is useful to carry out a Retrosynthetic Analysis of the route.

Work backwards from the target molecule to the starting material

Determine if each step is reasonable.

For synthesis dealing with Aromatic Rings, it is useful to keep in mind several things.

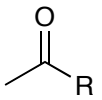
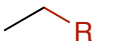
Which groups can be directly added to the ring

Which groups must be made by modification of other substituents

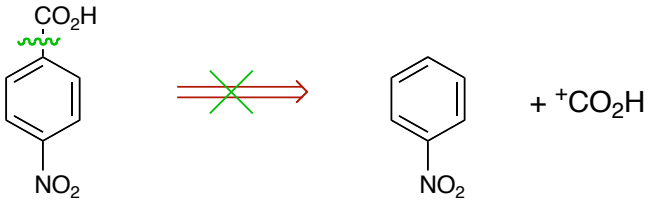
Activators, deactivators - o,p- or m- directors

For alkyl groups it is often best to do FC-Acylation followed by reduction

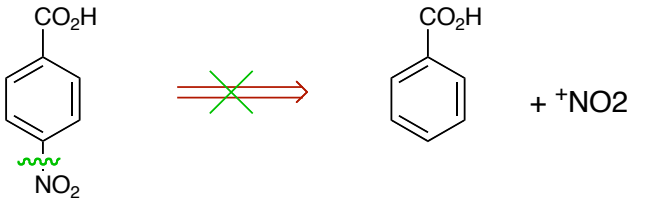
Aromatic Functionalization Chart

Substituents we can add directly		Substituent Modifications
—SO_3H		
—X	→	—OH
—NO_2	→	—NH_2
	→	 —CO_2H
—R	→	—CO_2H

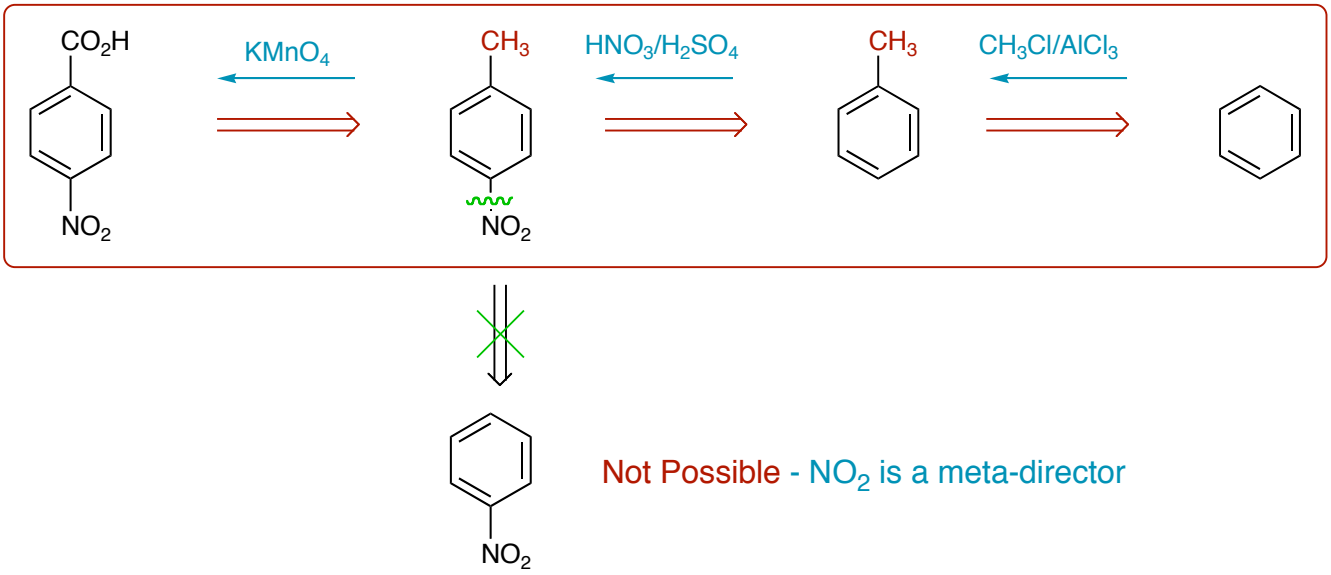
Retrosynthetic Analysis for how to synthesize p-nitrobenzoic acid

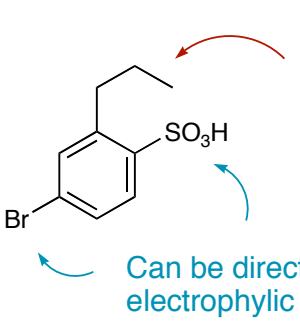


Not Possible - no way to add carboxylic acid directly. Also, NO_2 is a meta-directory, so anything you add would be in the wrong place.



Not Possible - you can add NO_2 with HNO_3/H_2SO_4, but the CO_2H group would be a meta director.





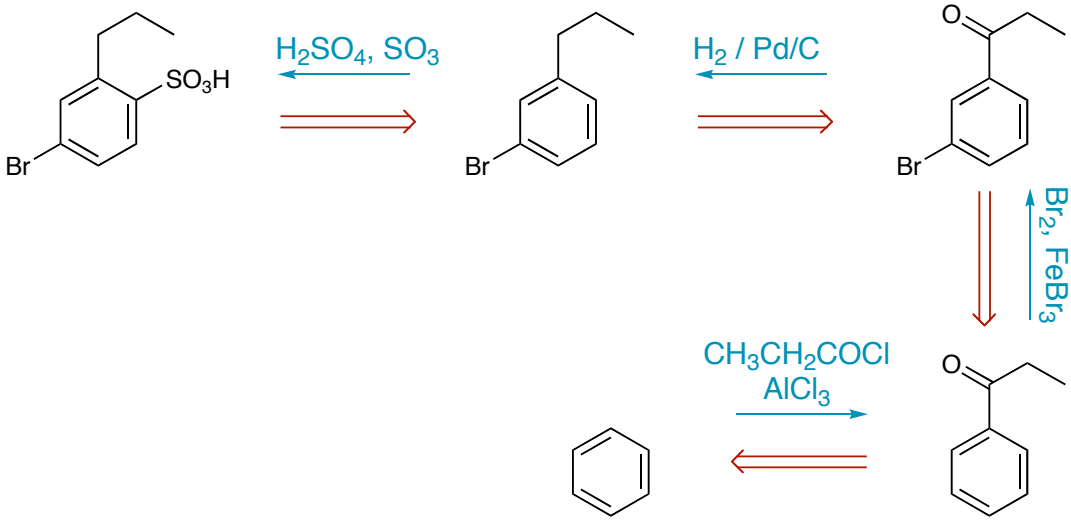
Due to carbocation rearrangements, need to use F-C Acylation first, then reduce the ketone to alkane

Can be directly added with electrophylic substitution

Steps needed to incorporate functional groups:

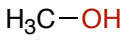
Br_2, $FeBr_3$
H_2SO_4, SO_3
CH_3CH_2COCl, $AlCl_3$
H_2 / Pd/C (to reduce ketone to alkane)

Retrosynthesis that would work for every step

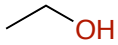


Naming

Alcohols are generally named by dropping the e, and adding ol. If required, the position of the OH group is given by numbering either before the name, or in the middle of the name. There are several common names that are used for alcohols.

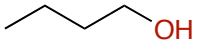


methanol
(methyl alchol)

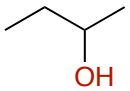


ethanol
(ethyl alcohol)

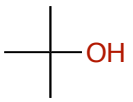
2-propanol
(isopropanol)



1-butanol
(*n*-butanol)

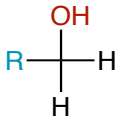


2-butanol
(*sec*-butanol)

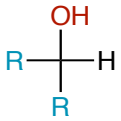


tert-butanol

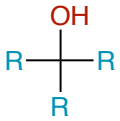
Alcohols are classified according to their degree of alkyl substitution.



1° - primary



2° - secondary



3° - tertiary