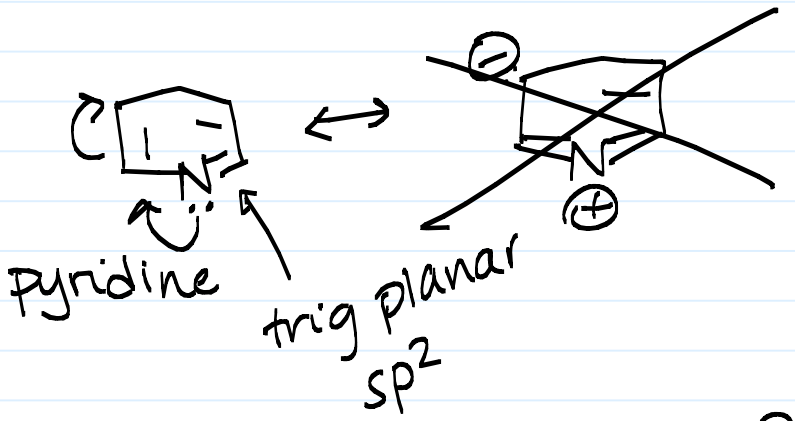
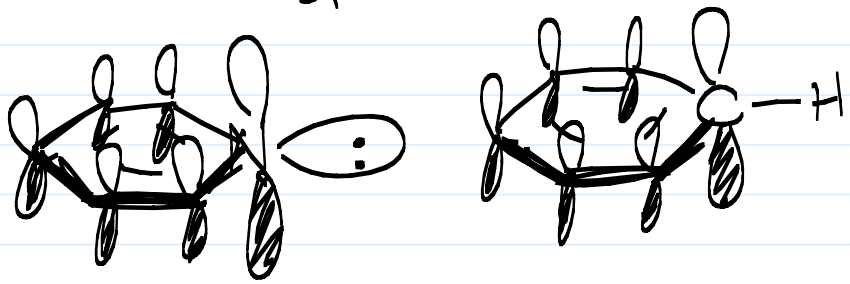
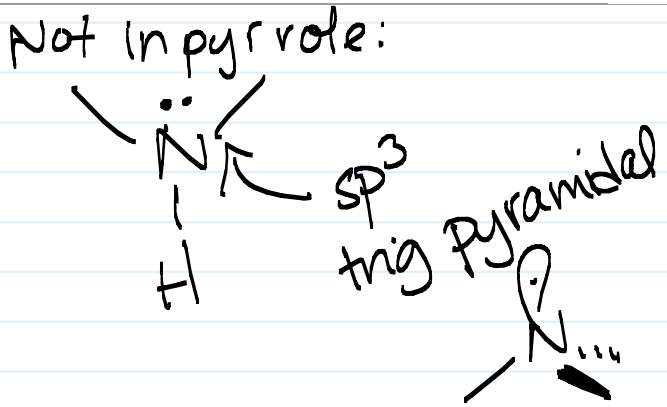
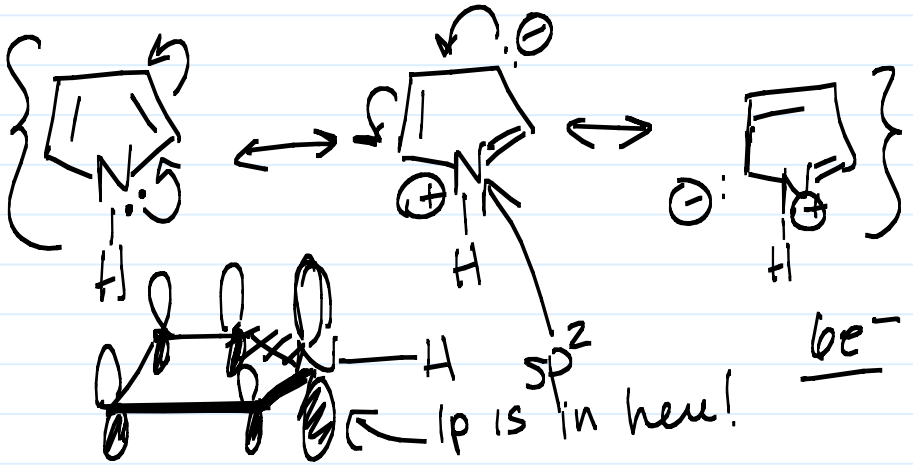
More Aromaticity (Lecture 3, 2/20/14)

Note Title 2/20/2014





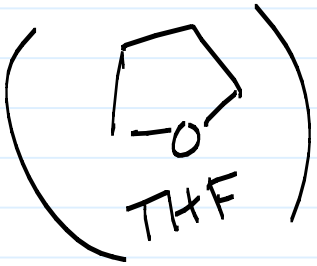




furan

1) cyclic ✓

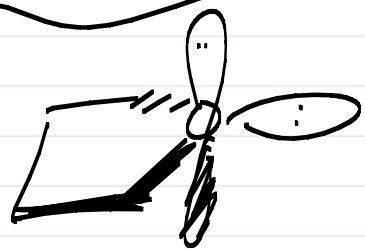
2) fully conjugated? ✓



3) planar ✓

4) $2\pi = 4e^-$

$lp_O = \frac{2e^-}{6e^-} = 4n+2, n=1$



quinoline

1) cyclic ✓

2) fully conj ✓

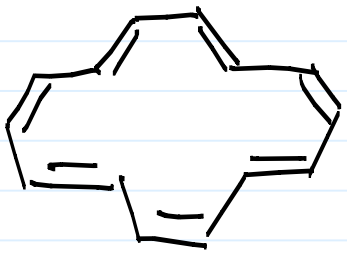
3) planar ✓

4) 10 e⁻ = 4n+2 ; n=2 ✓

Annulenes

[6]-annulene

[14]-annulene



1) cyclic ✓
2) fully conj ✓
3) planar ? ✓
4) $14e^- = 4n+2$
$n = 3$ ✓

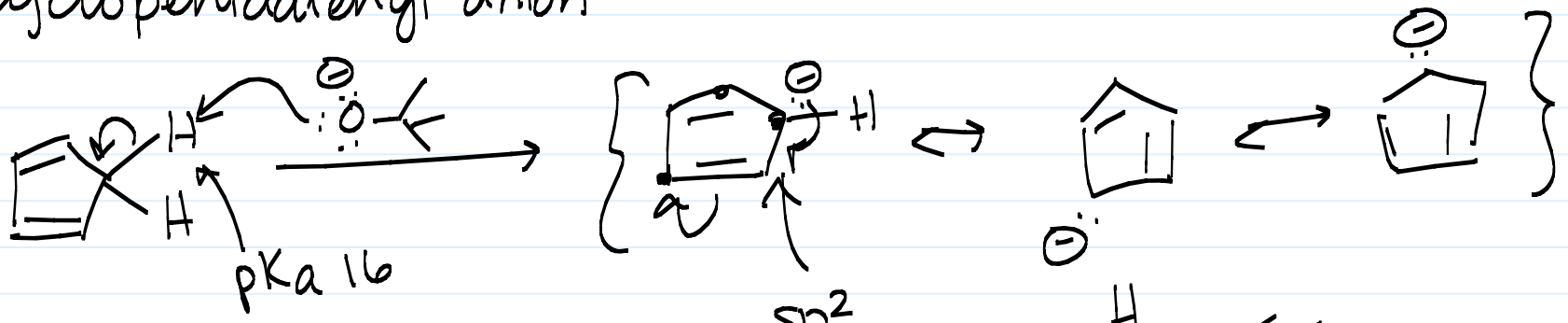
[10]-annulene

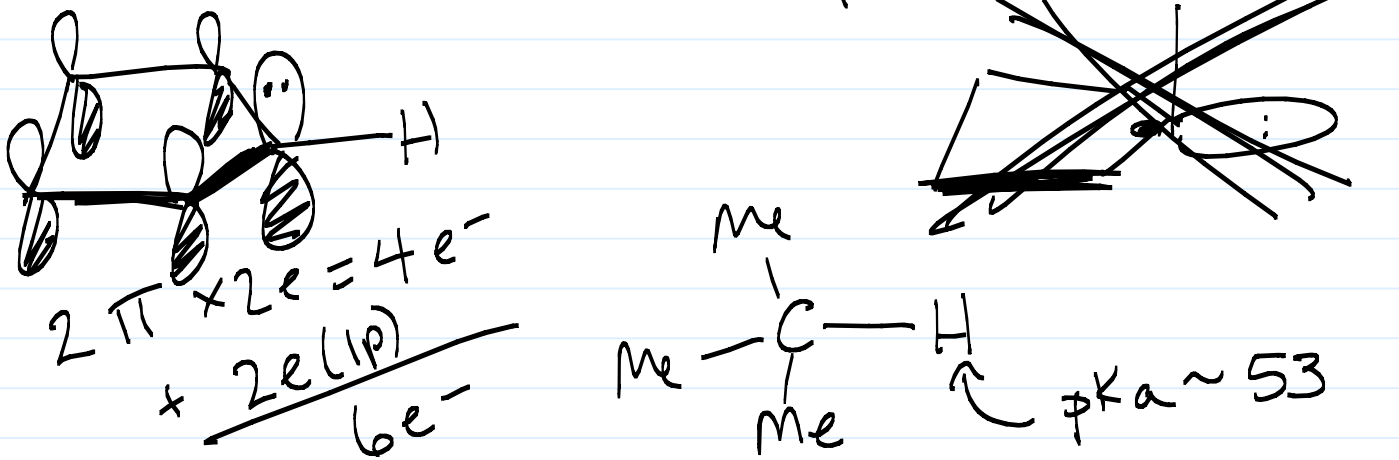
Not planar!

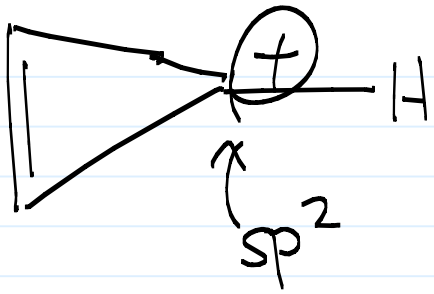
Not aromatic!

Aromatic Ions

1) Cyclopentadienyl anion





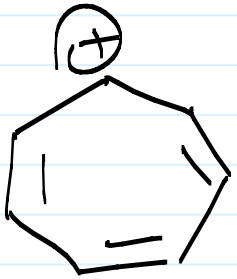


1) cyclic ✓

2) conj ✓

3) planar ✓

4) $2e^- = 4n+2$, $n=0$ ✓

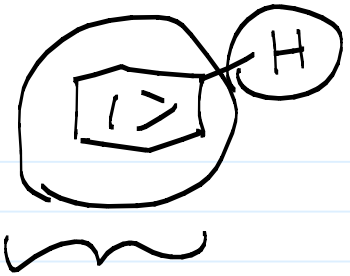


tropylium cation

Also aromatic ✓

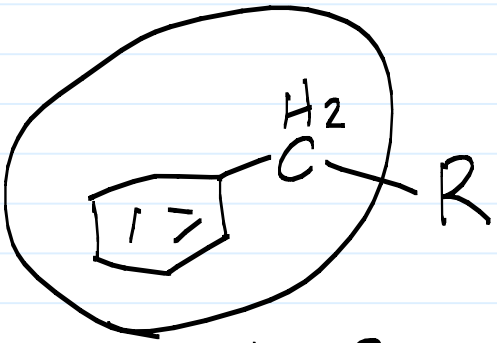
Nomenclature

Substituted benzenes

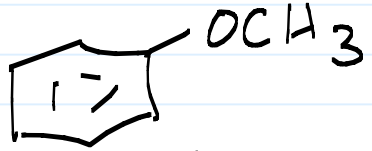


= Ph-H

phenyl = Ph = C_6H_5

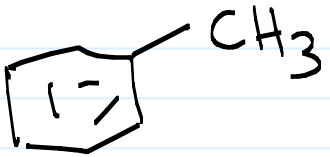


Benzyl = Bn

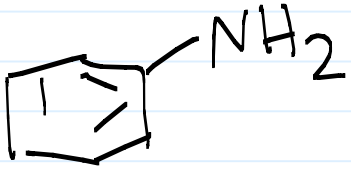


= Ph-OCH_3

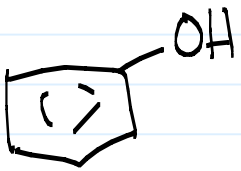
anisole



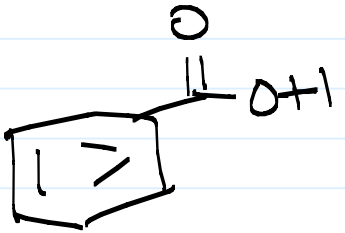
toluene
PhMe



aniline

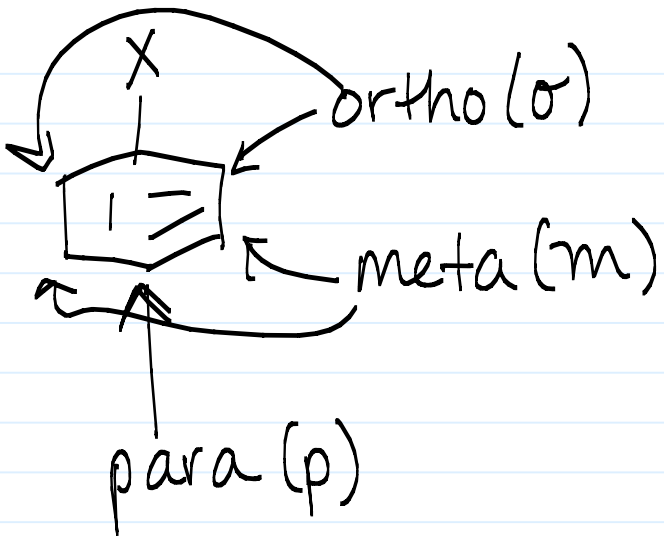


phenol

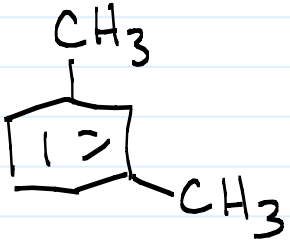


benzoic acid

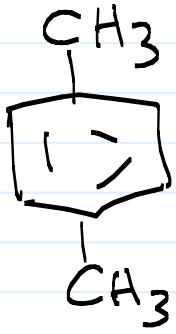
Disubstituted:



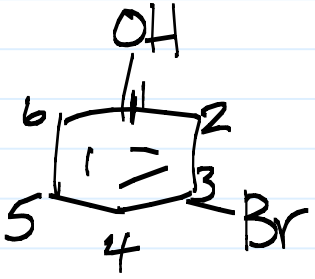
o, m, p = denote relative position w.r.t. X



m-xylene



p-xylene

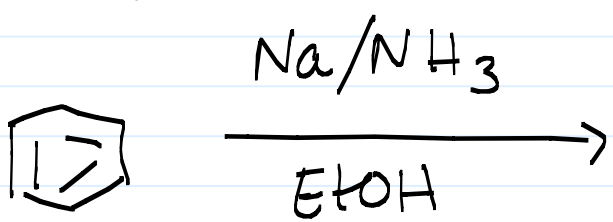


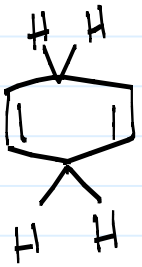
m-bromophenol

3-bromophenol

Reactions of Benzene Derivatives:

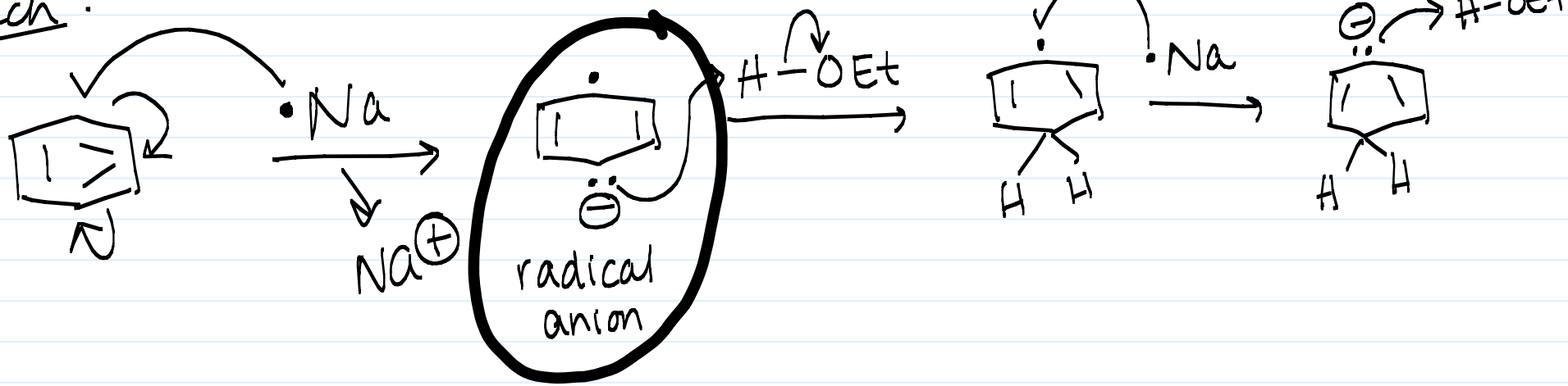
1) Birch Reduction:





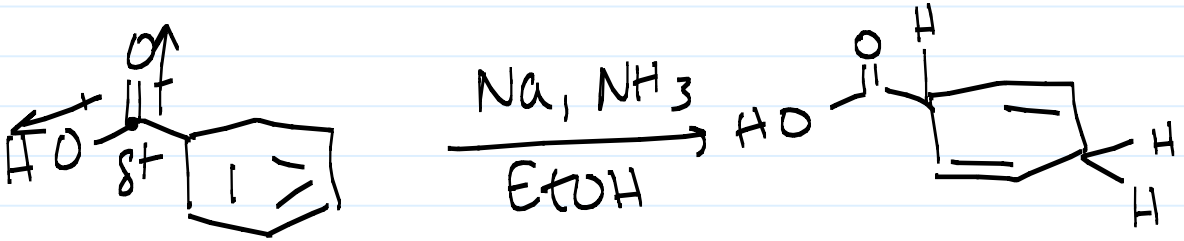
diene

Mech:



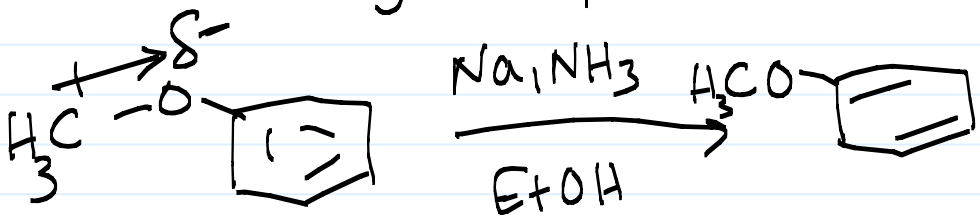
Substituent Effects

1) Electron-withdrawing Groups (EWG)



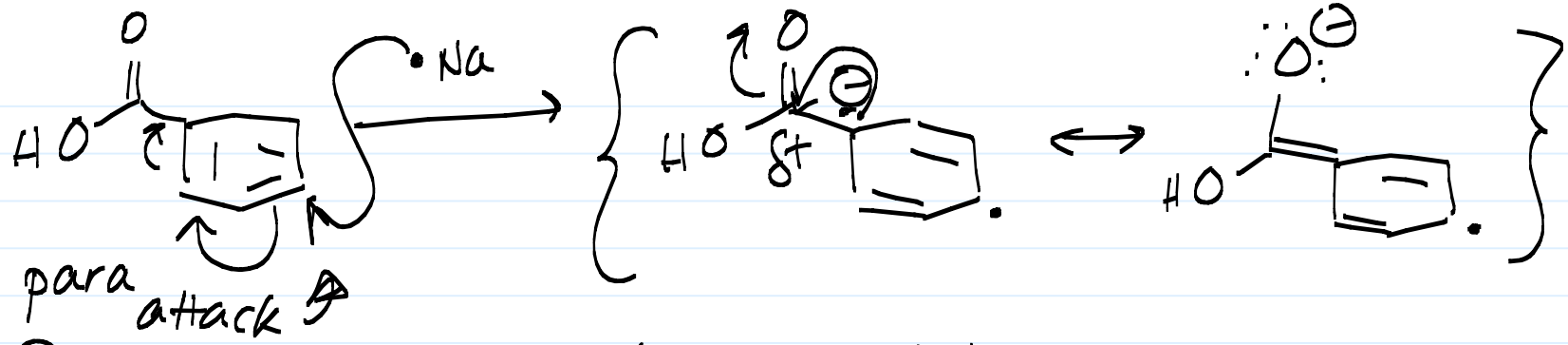
EWG ends up between double bonds.

2) Electron-donating Group (EDG)



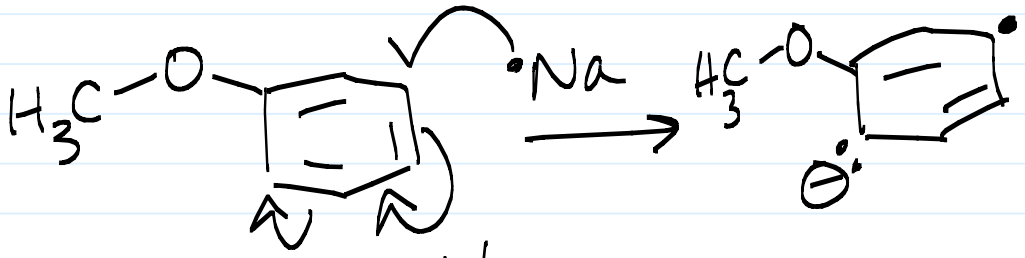
EDG ends up on double bond.

EWG



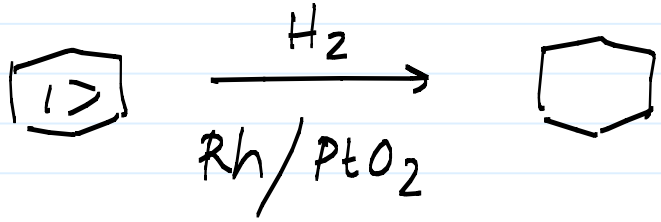
⊖ is stabilized by being next to δ+ of EWG.

EDG

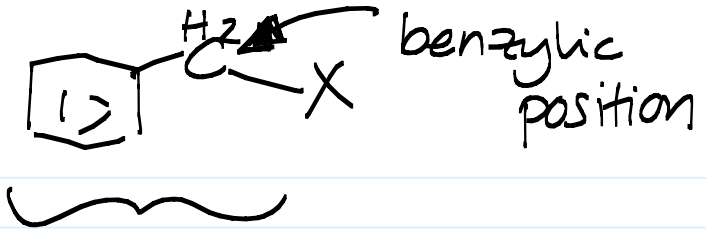


⊖ does not want to be next to EDG

2) Total Reduction of Benzene: "Super" Catalyst:

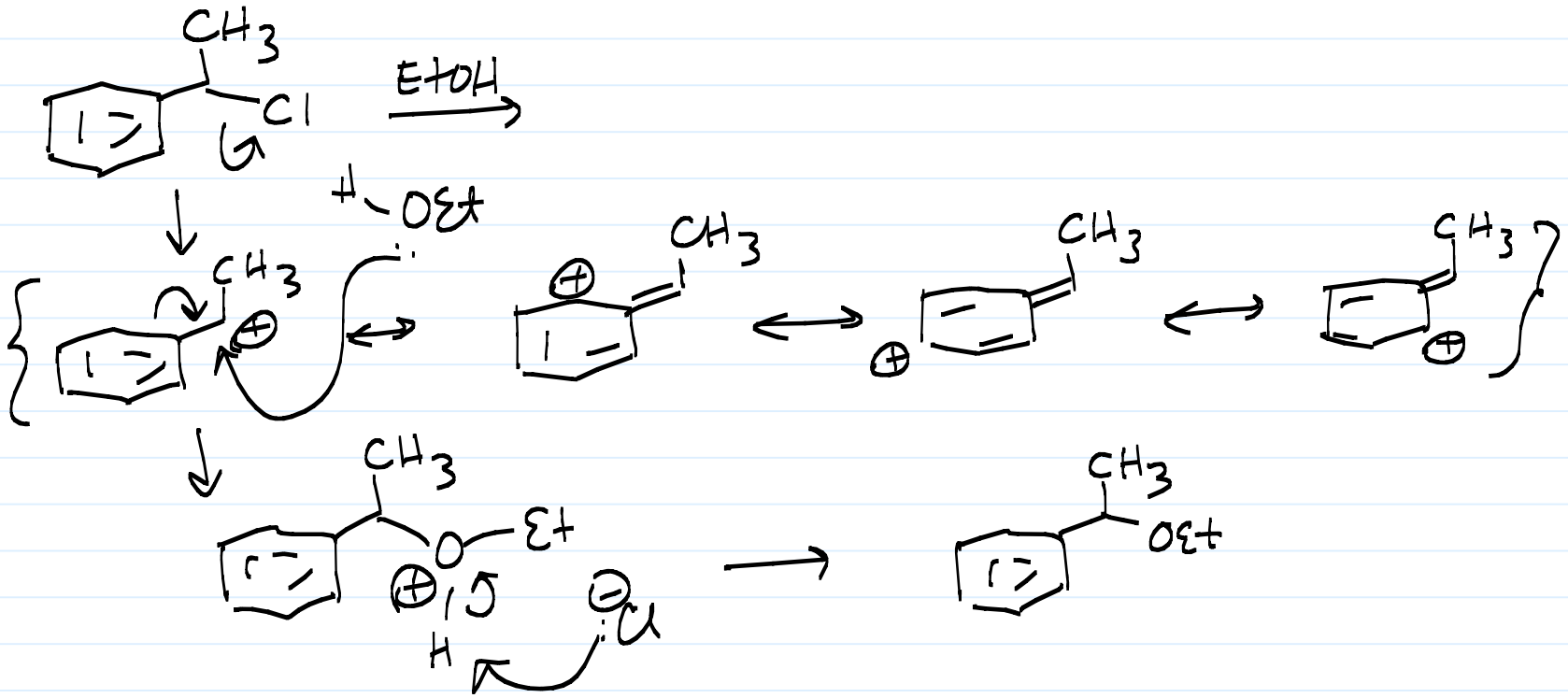


3) Reactions @ Benzylic Position:

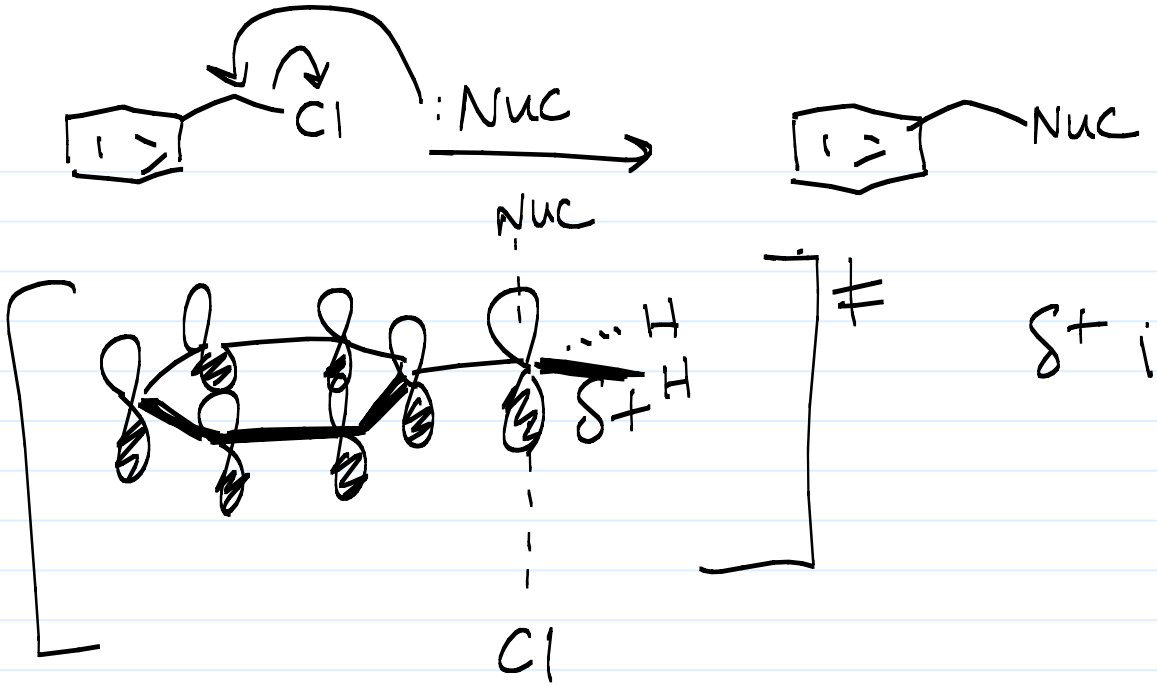


↳ fast & facile

a) S_N1



b) S_N2 :



δ+ is delocalized.