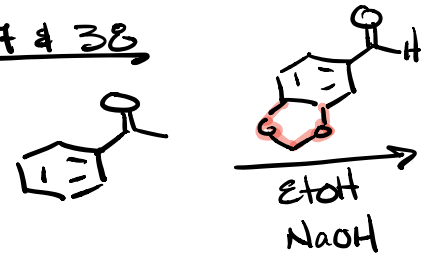
Michael-Aldol Rxn

Exp 64 in Pavia 5th ed p. 564

Relates to Exp. 37 & 38 in Pavia

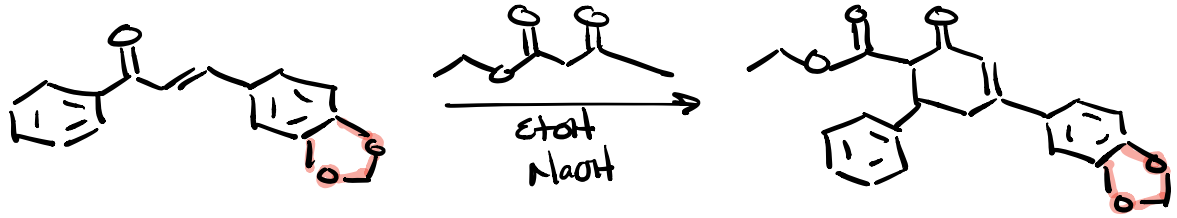
\# 37 & 38

37

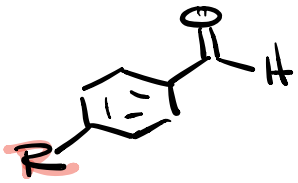


Chalcone

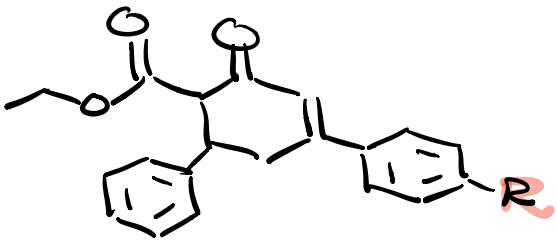
38



Exp 64

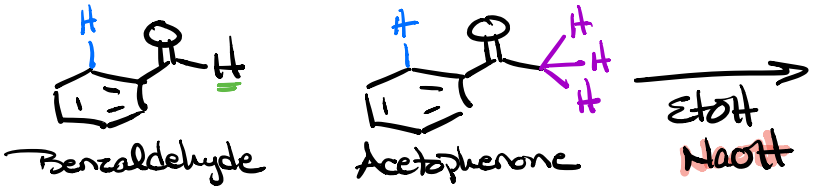


R
-Cl
$-O-CH_3$
$-NO_2$
$-CH_3$



Make 1 mmol

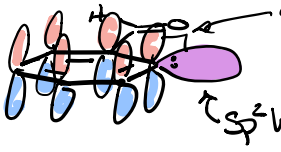
Aldol Mechanism



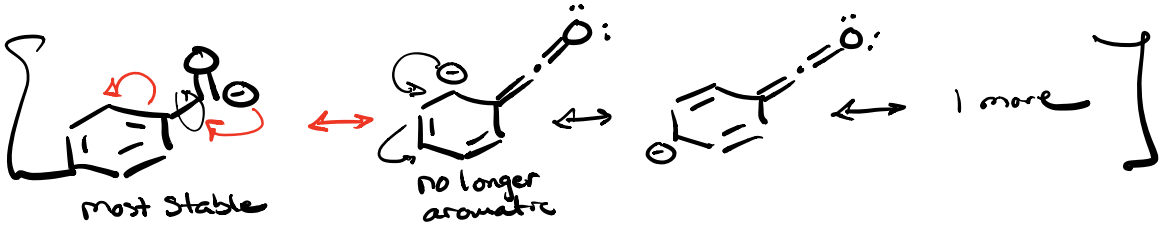
1st Look for acidic proton

most stable ? ⇒ most acidic proton

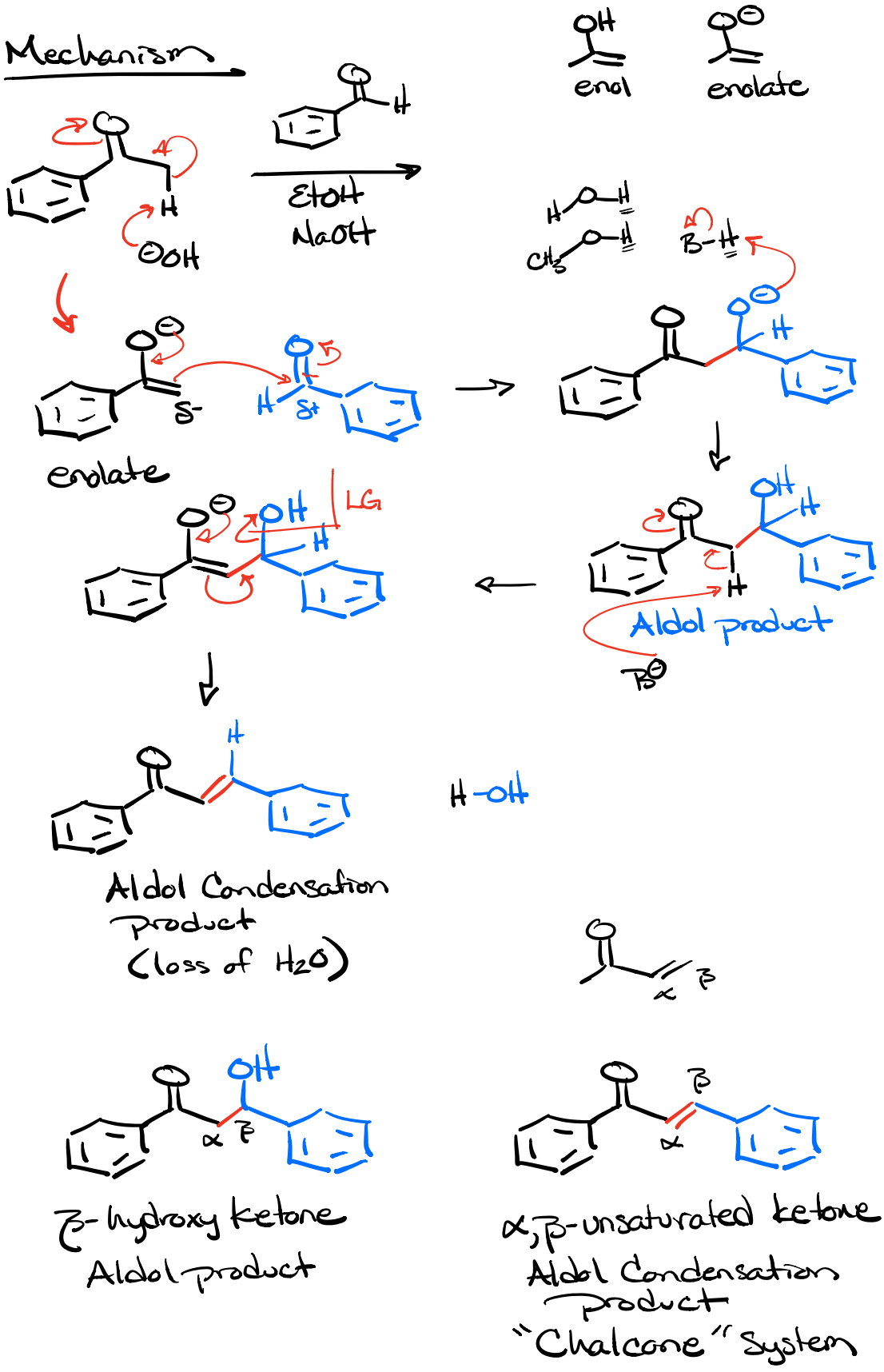
A



B

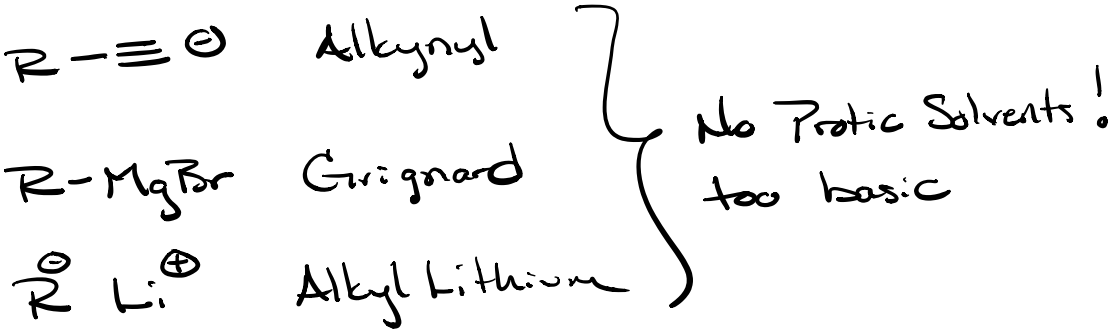


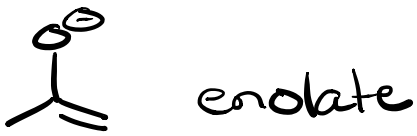
C

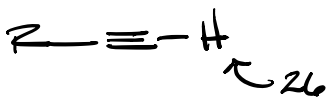

Mechanism
EtOH
NaOH
enol
enolate
enolate
LG
Aldol product
H-OH
Aldol Condensation
product
(loss of H2O)
β-hydroxy ketone
Aldol product
α,β-unsaturated ketone
Aldol Condensation
product
"Chalcone" System

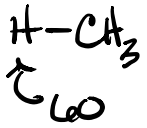
Enolate as nucleophile

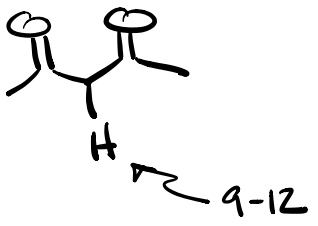
C⁻ nucleophiles

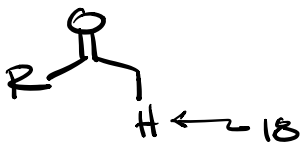


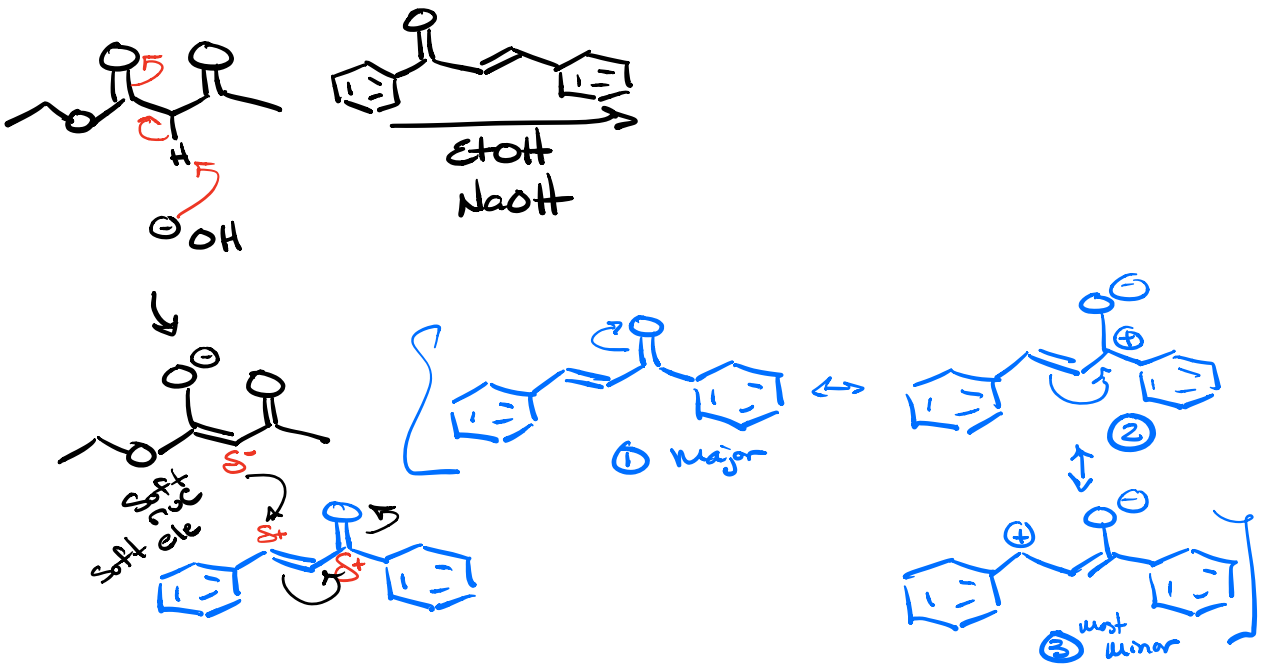


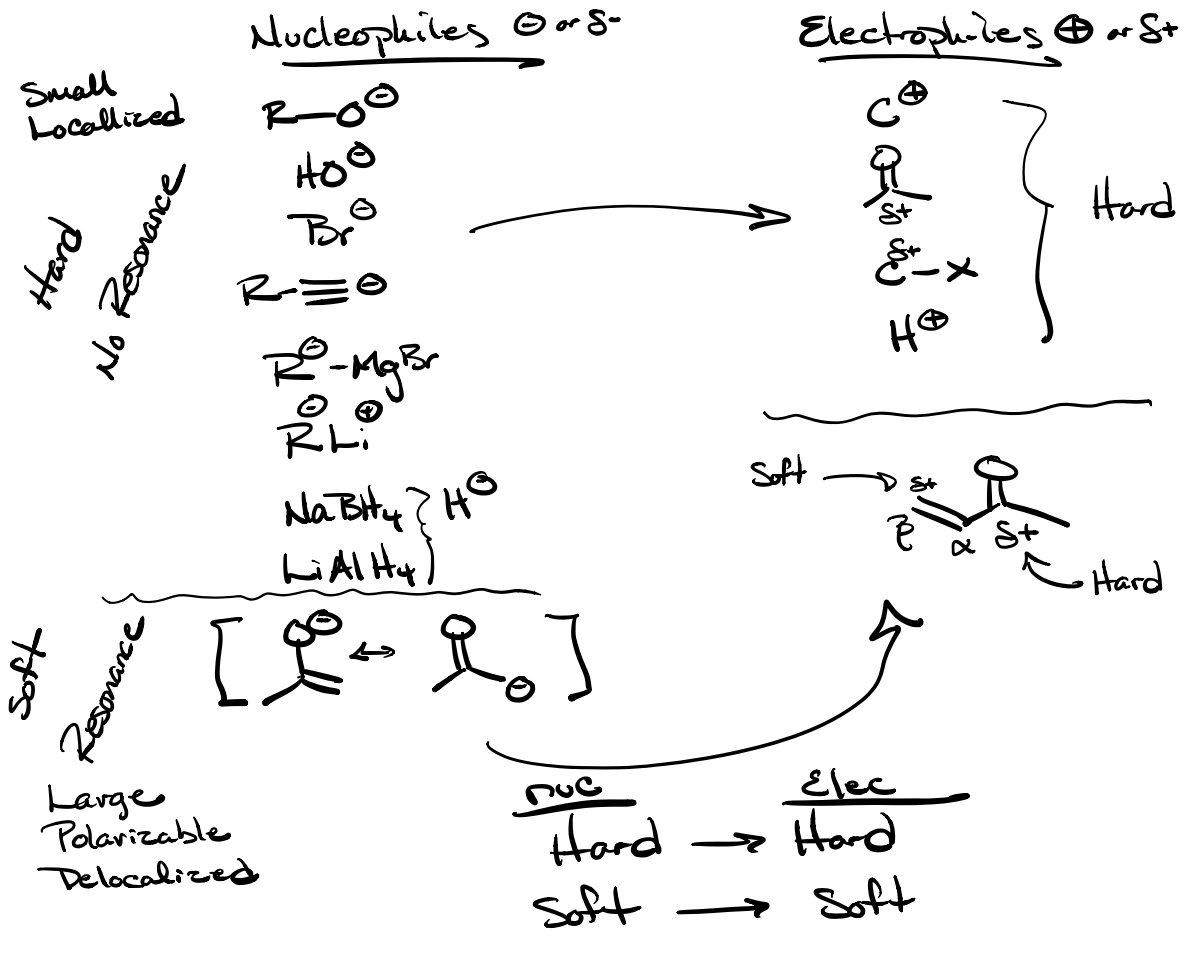


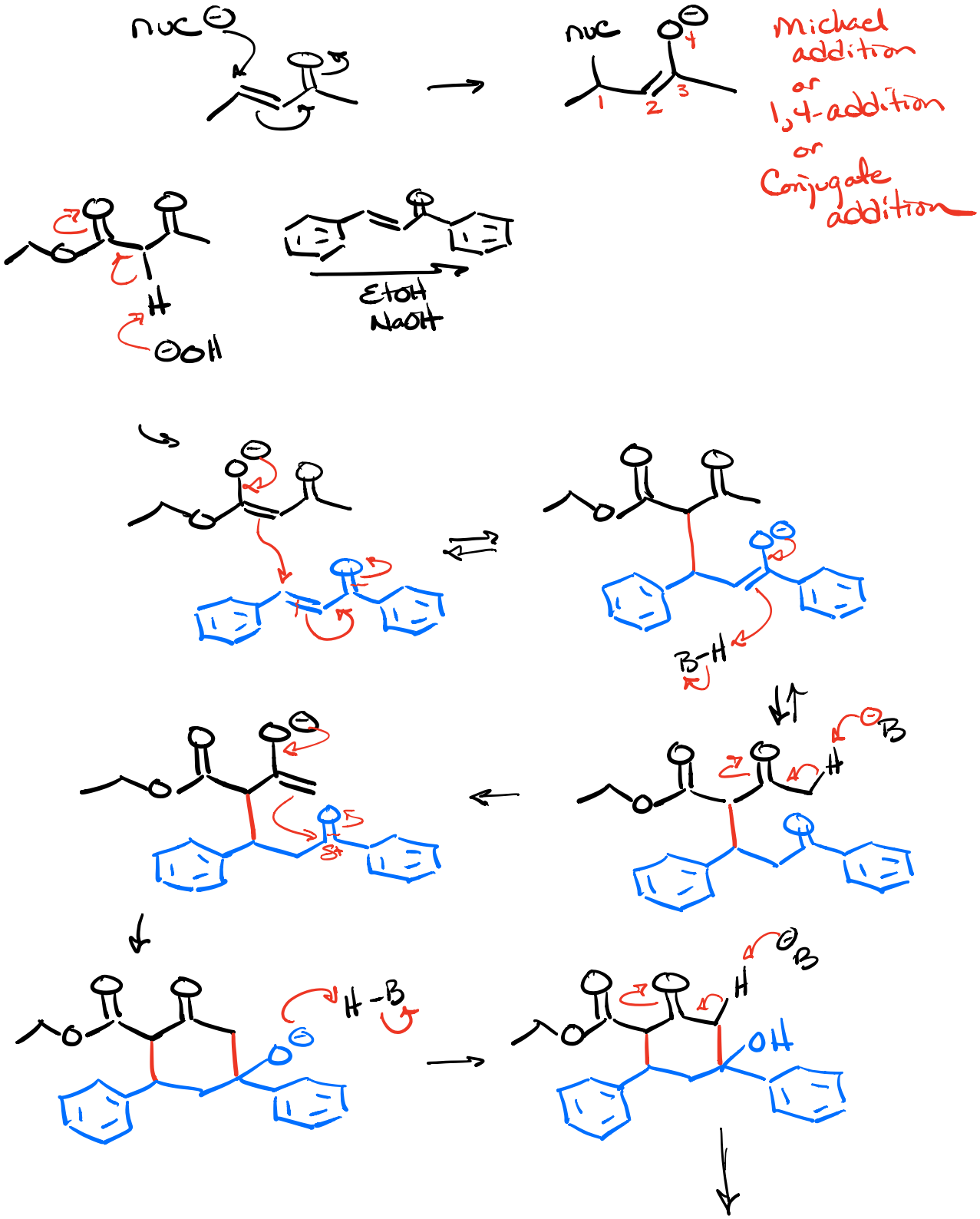


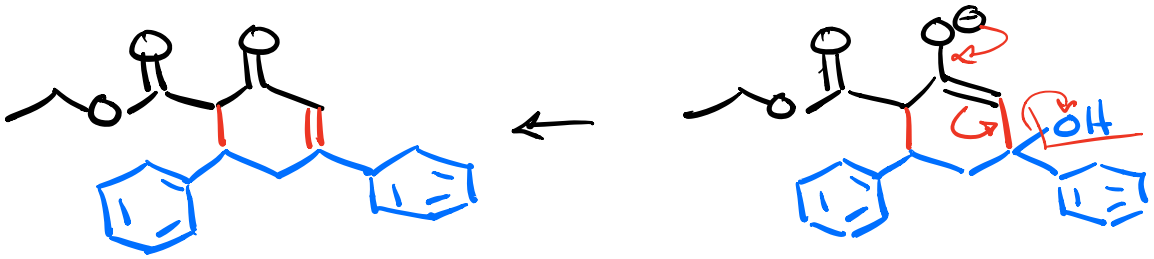




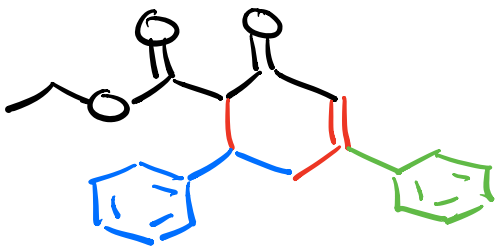

EtOH
NaOH
Soft nuc
Soft ele
major
most minor

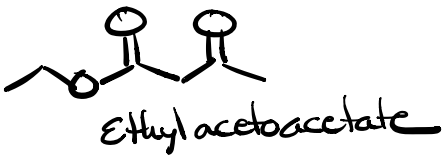

Nucleophiles ⊖ or δ-
Electrophiles ⊕ or δ+
Small
Localized
Hard
No Resonance
Hard
Soft
Resonance
Large
Polarizable
Delocalized
Soft
Hard
nuc
elec
Hard → Hard
Soft → Soft


nuc
nuc
1
2
3
4
Michael addition
or
1,4-addition
or
Conjugate addition
EtOH
NaOH
OOH
B-H
H-B
OH

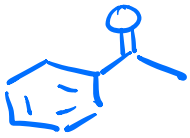


final product

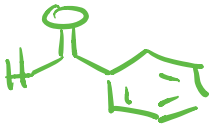




Ethyl acetoacetate

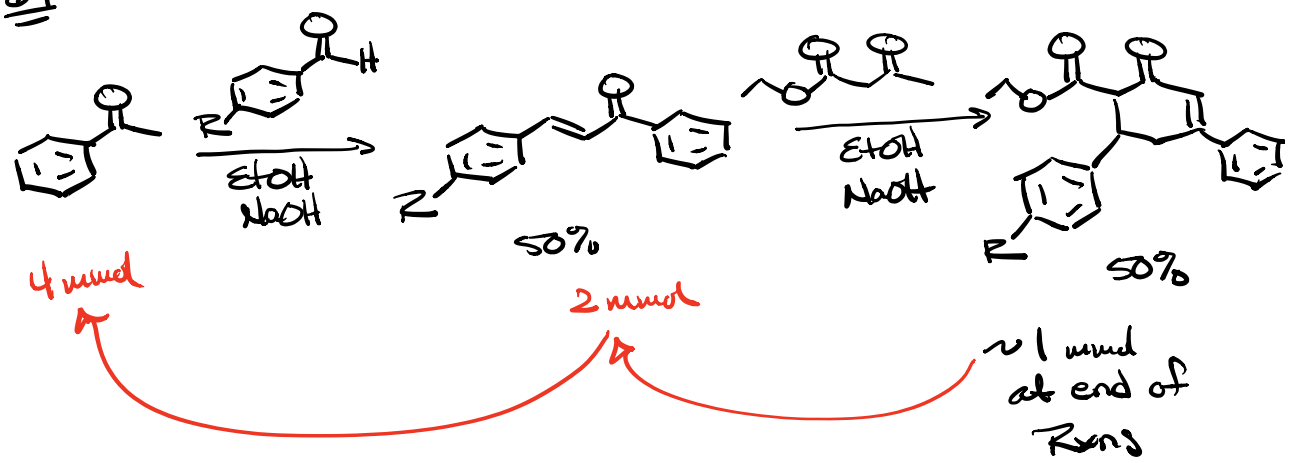


Acetophenone

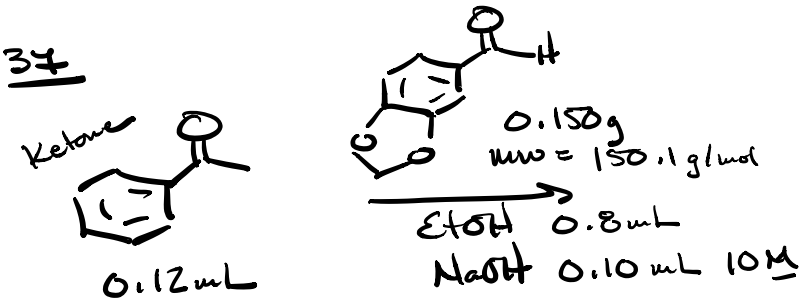


Benzaldehyde

64



37



(MW = 120.2 g/mol d = 1.03 g/mL)

How big was this Reaction?

$$0.12\,\text{mL ketone} \times \frac{1.03\,\text{g}}{1\,\text{mL}} \times \frac{1\,\text{mol}}{120.2\,\text{g}} \times \frac{1000\,\text{mmol}}{1\,\text{mol}}$$

$$= 1.03\,\text{mmol} \sim 1\,\text{mmol}$$

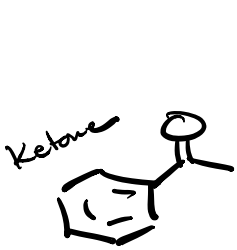
slight excess of ketone over aldehyde

$$0.150\,\text{g Aldehyde} \times \frac{1\,\text{mol}}{150.1\,\text{g}} \times \frac{1000\,\text{mmol}}{1\,\text{mol}} = 0.999\,\text{mmol}$$

$$\sim 1\,\text{mmol}$$

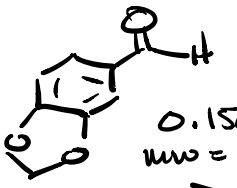
Scale up by factor of 4

mult everything by 4



4 x 0.12mL

(MW = 120.2 g/mol d = 1.03 g/mL)



0.150g x4

MW = 150.1 g/mol

EtOH 0.8mL x4

NaOH 0.10 mL 10M x4

Work up

4x add 2mL 0°C DI H_2O to Round bottom

.48 mL
.60 mL
3.2 mL
.40 mL
8.0 mL

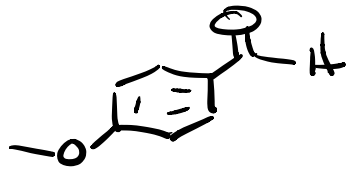
12.68 mL total volume

~13mL

RB

10mL
25mL
50 mL
100 mL
250 mL
500 mL

* Golden Rule
⇒ Never fill more than 50%

①  Data for this in Exp 64

use Exp 37 as model
Scale 4x
write out produre

② Also Scale Exp 38 using our wirk here as a model