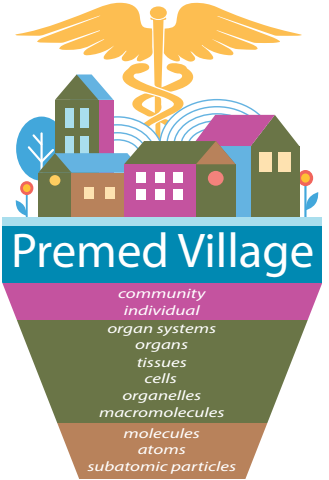

Organic Notes

premedvillage.com

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Stereoisomerism

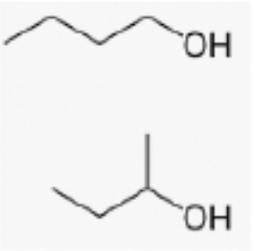
Isomers

tautomers - constitutional isomers that interconvert

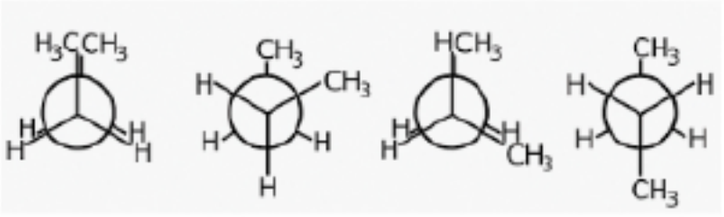
different connectivity

Stereoisomers

Constitutional



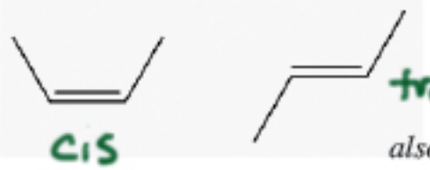
Conformational



conformations of butane

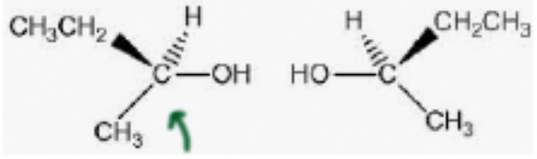
Optical

Geometric



also technically diastereomers

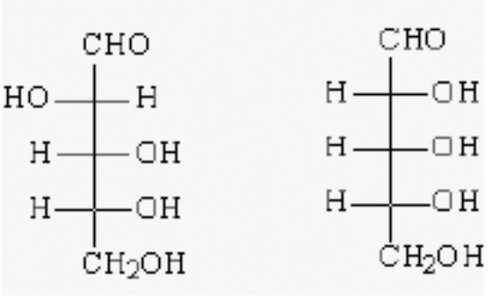
Enantiomers



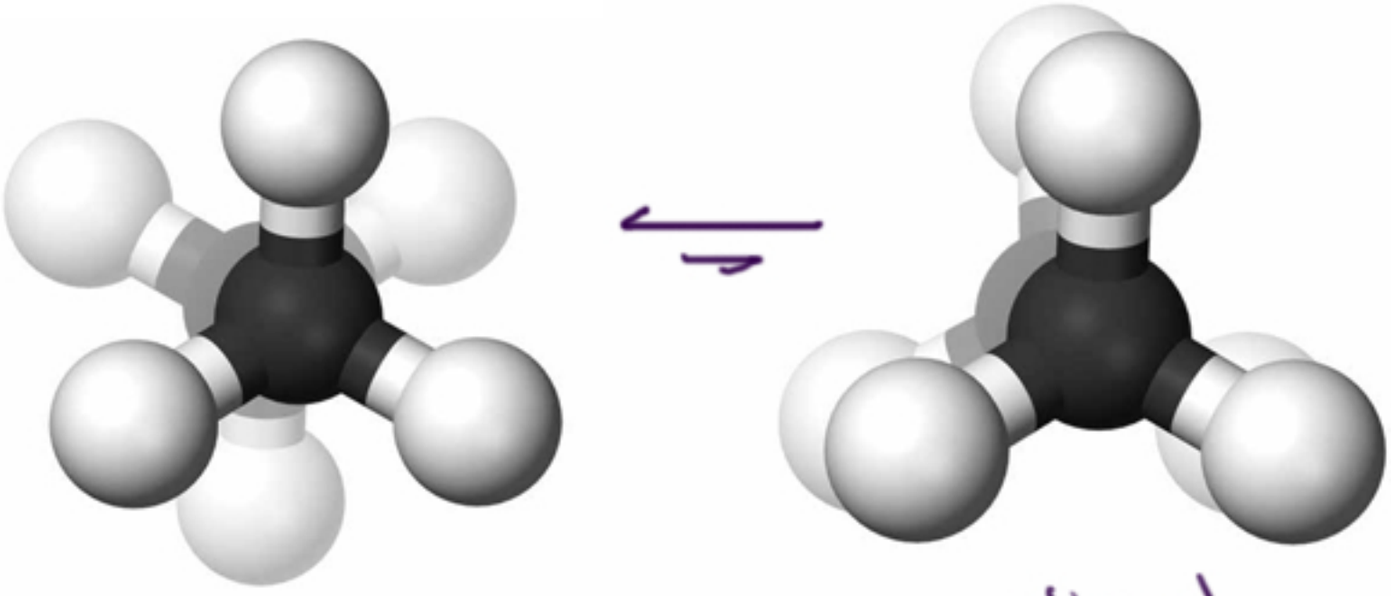
chiral center

non superimposable mirror images

Diastereomers



Conformational isomerism

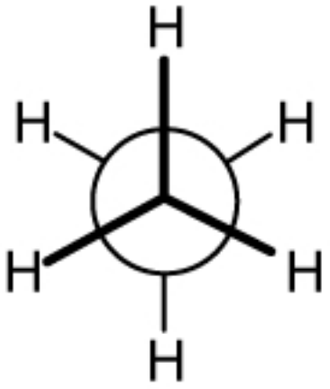


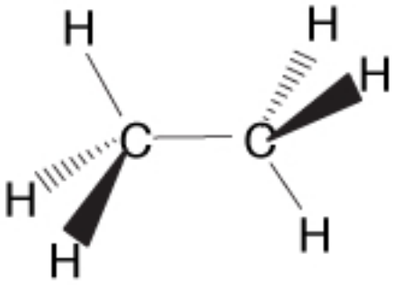
staggered

eclipsed

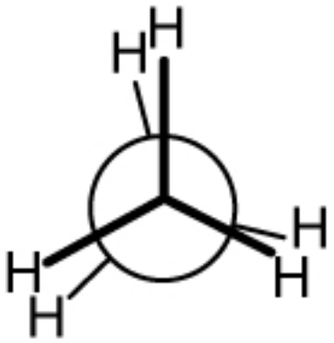
CH_3CH_3

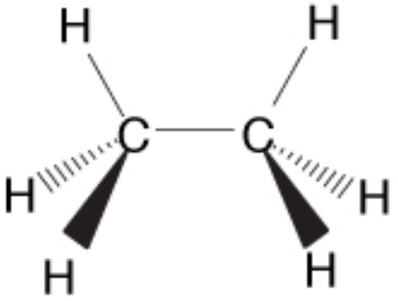
$$K = e^{-\Delta G^\circ / RT}$$



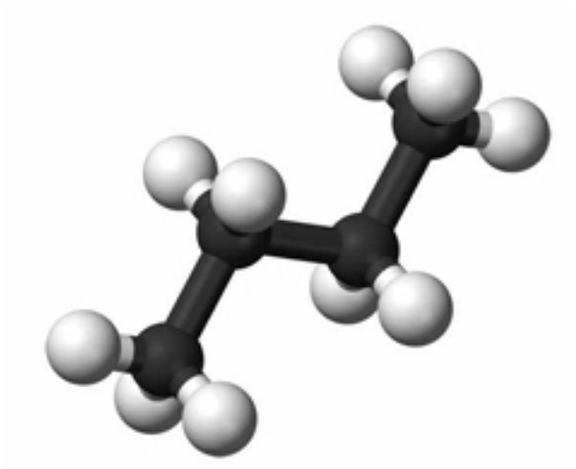


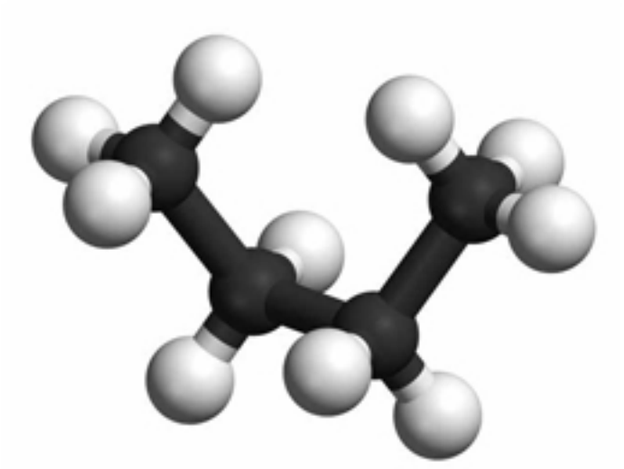
Conformations of ethane

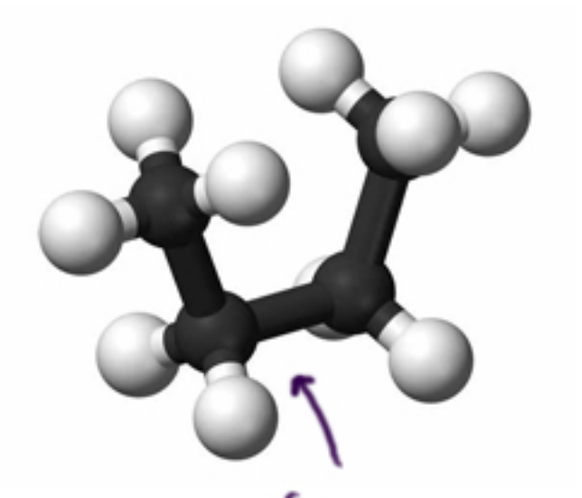




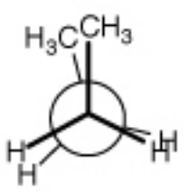
Conformations of butane

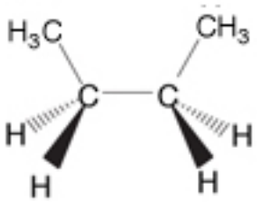




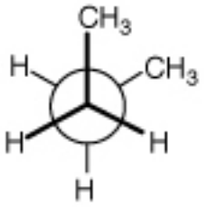


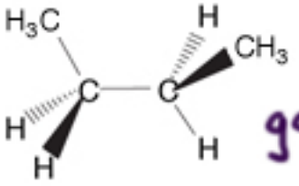
free rotation



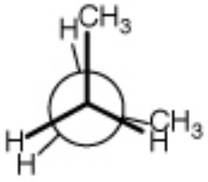


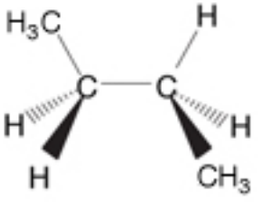
methyl eclipsed



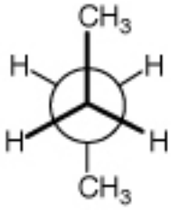


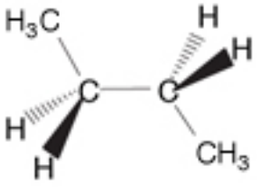
gauche



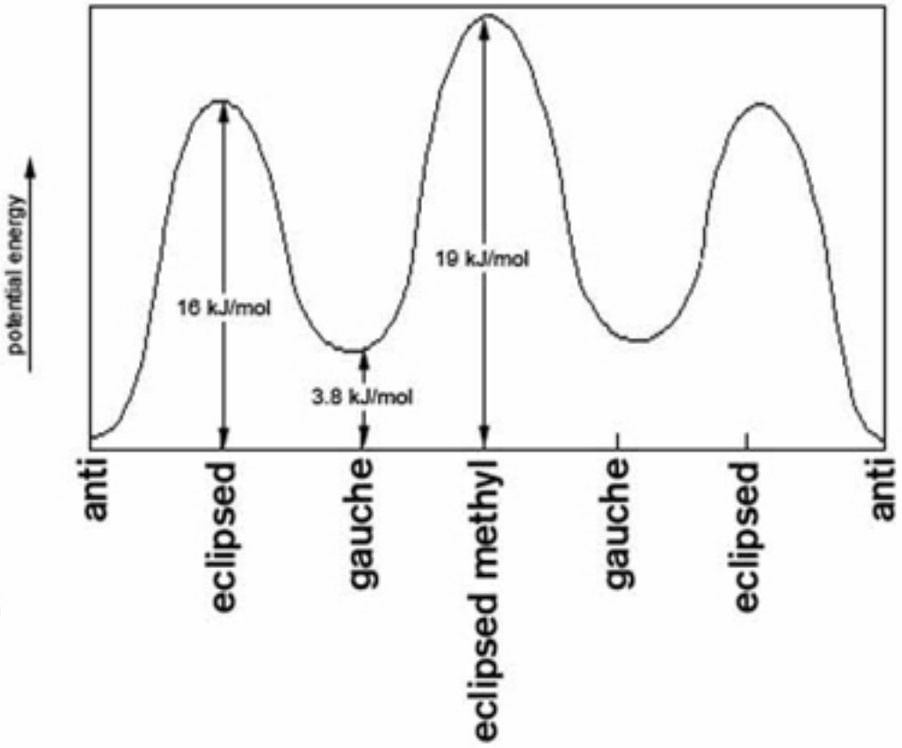


eclipsed





anti



eclipsed methyl $\longrightarrow$ anti

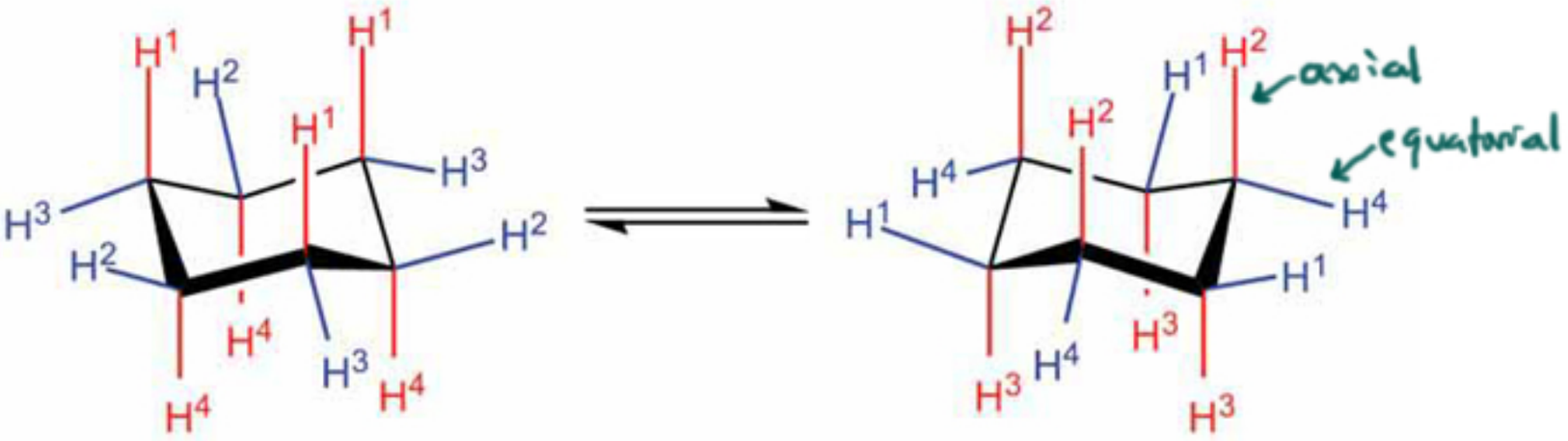
$\Delta G^\circ = -20\ kJ/mol$

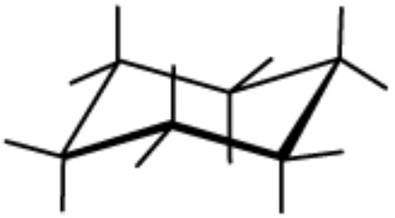
$K = \frac{[B]}{[A]}$ $K = e^{-\Delta G^\circ/RT}$

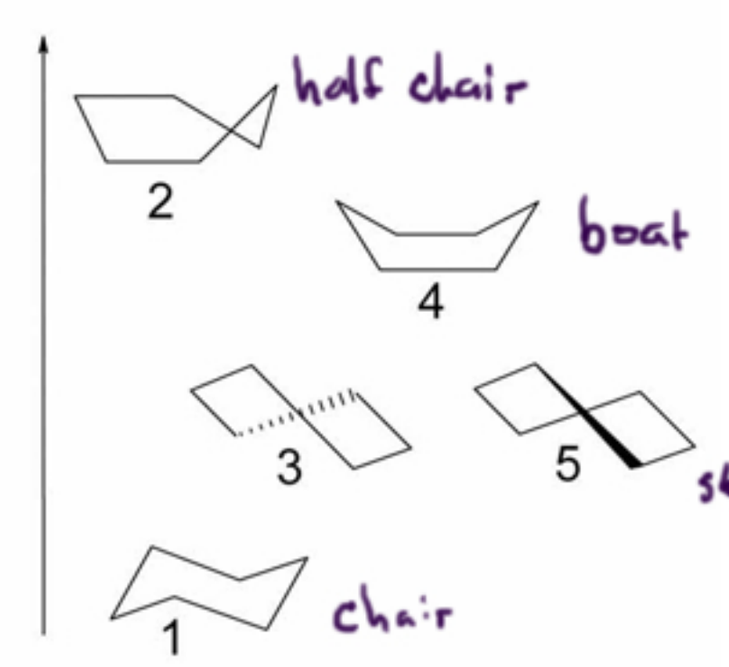
$K = e^{+20{,}000/(8)(300)}$

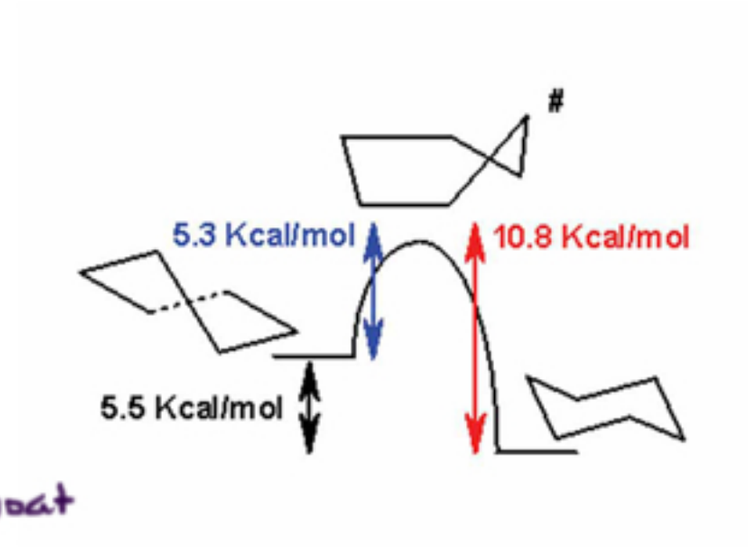
$\sim e^{8} \sim 500$

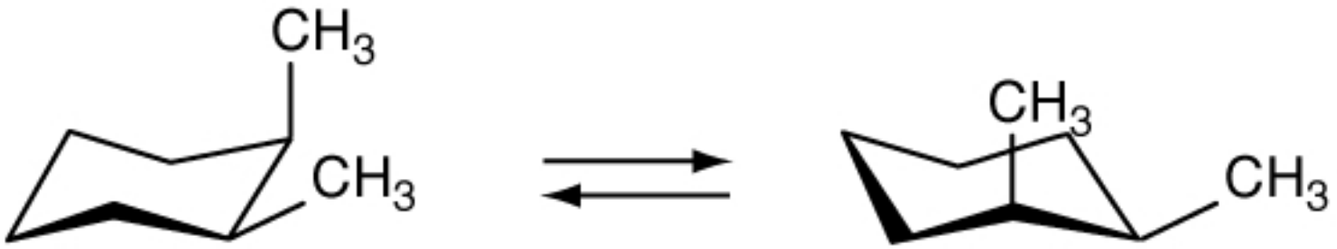
Ring flipping in cyclohexane

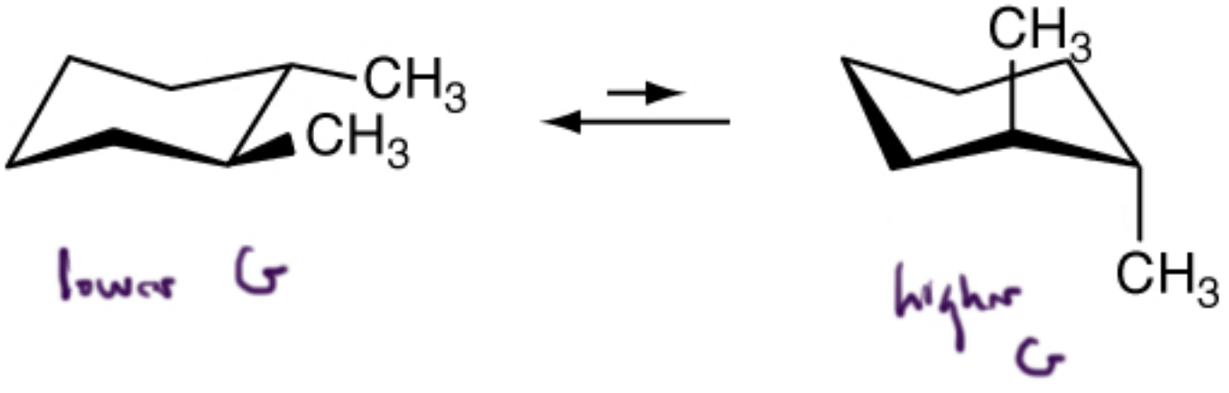


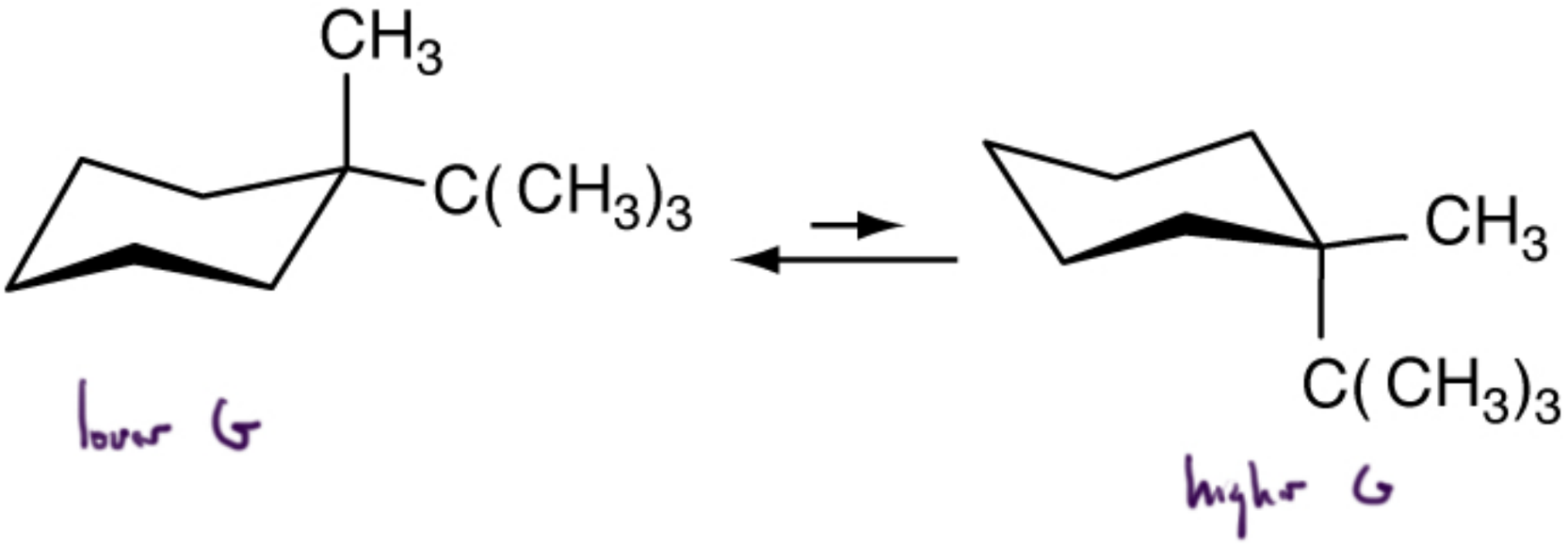



half chair
2
boat
4
3
5
skew boat
1
chair


#
5.3 Kcal/mol
10.8 Kcal/mol
5.5 Kcal/mol

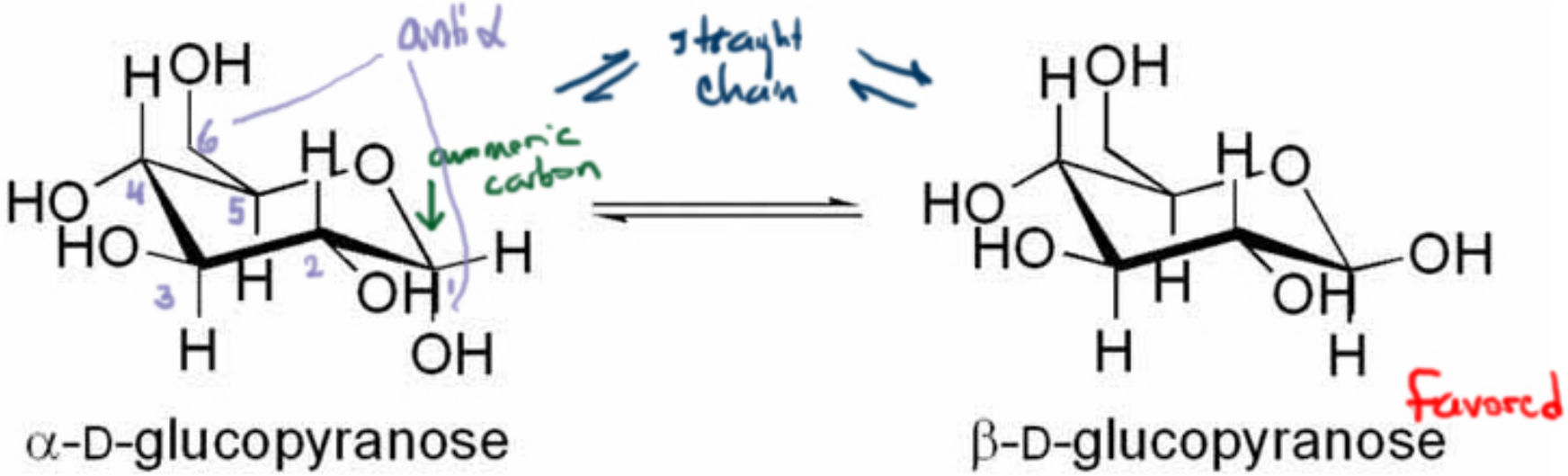

CH3
CH3
CH3
CH3


CH3
CH3
CH3
CH3
lower G
higher G



lower G

higher G

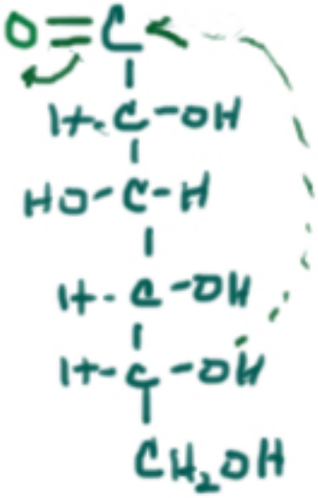


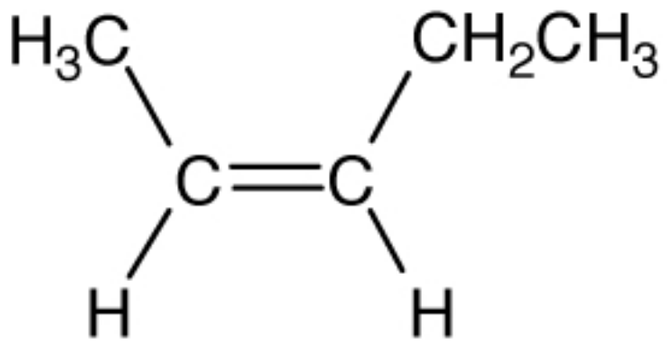
α-D-glucopyranose

β-D-glucopyranose

pyranose means 6 membered ring

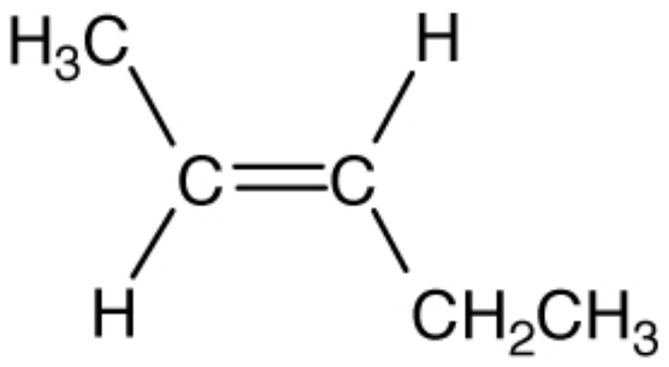
same as β-D-glucose





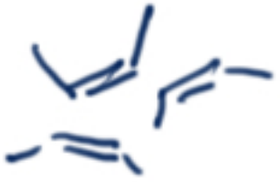
higher G

cis



trans

higher melting point

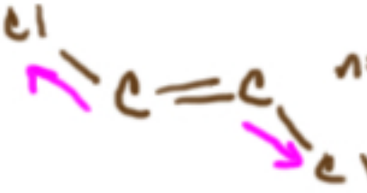


more access for van der Waals

However

dipole dipole

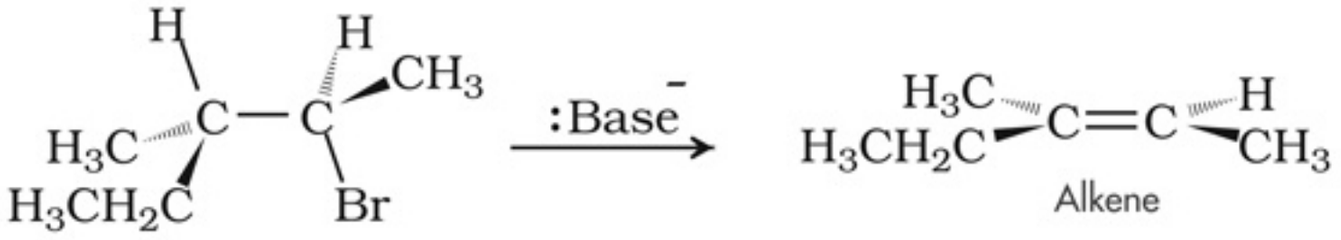
higher melting



no net dipole moment

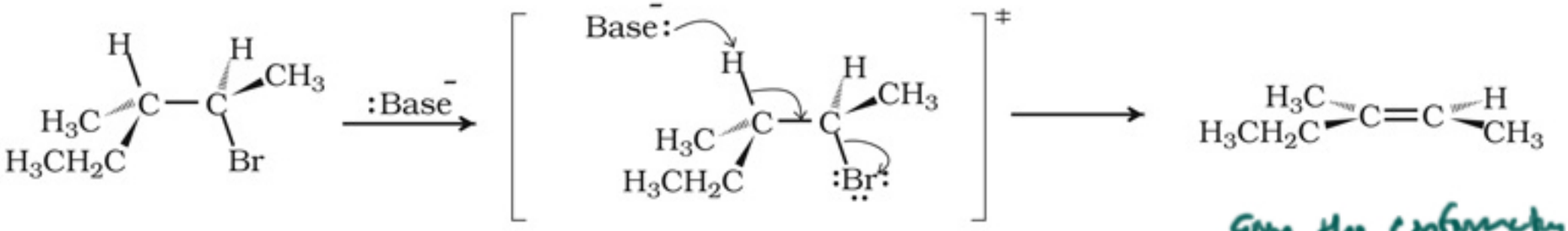
only Van der Waals

E2



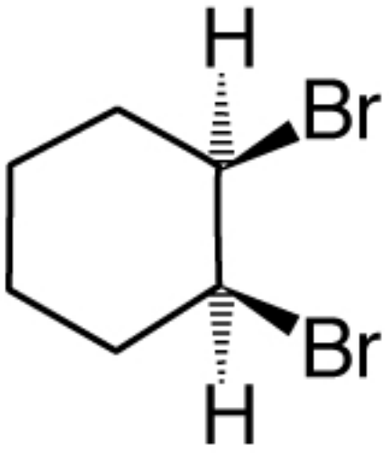
Alkyl halide

Alkene

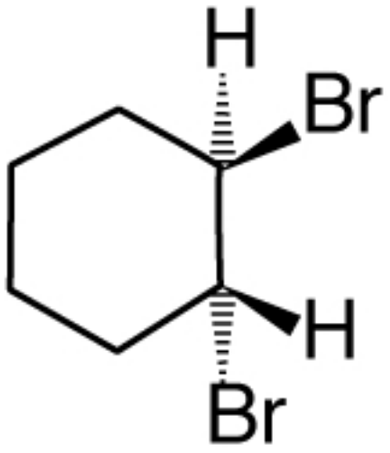


anti periplanar transition state

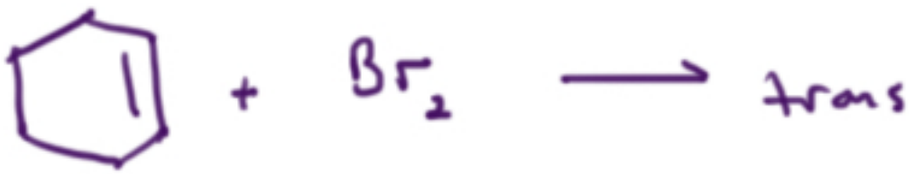
Given the conformation of the reagent, this reaction is stereospecific for cis product

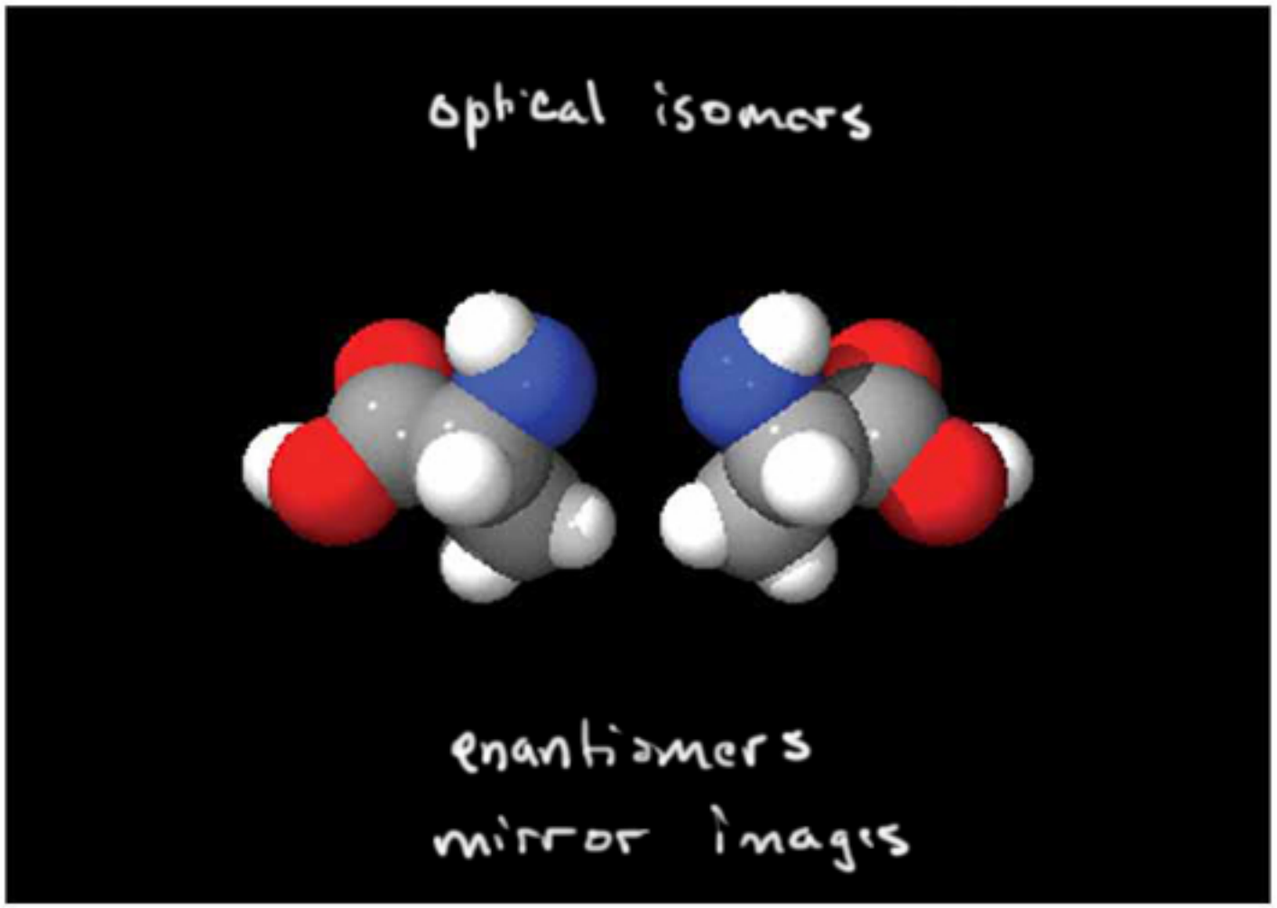


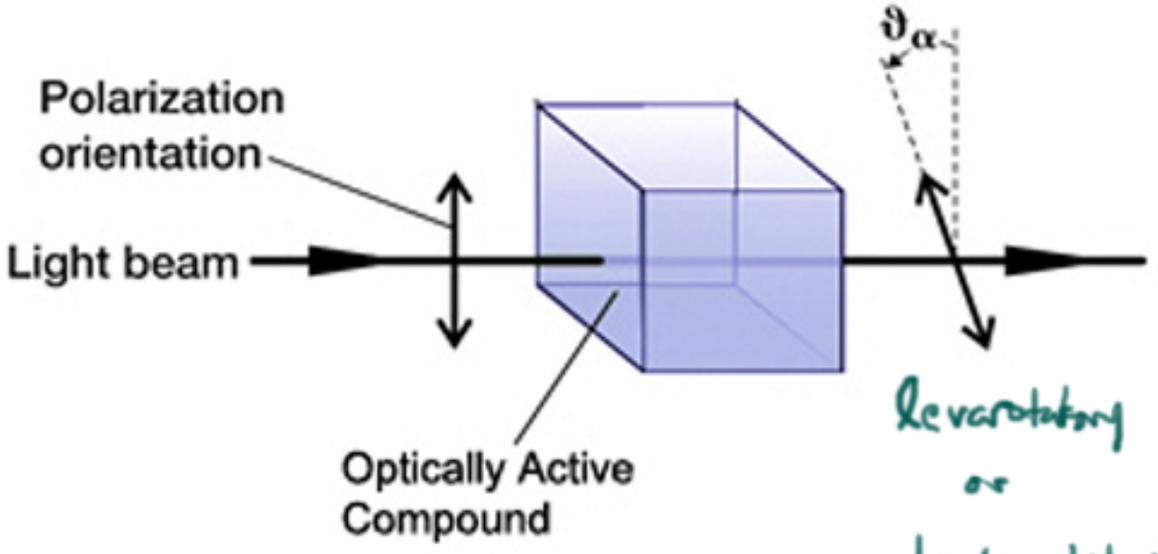
cis



trans




optical isomers
enantiomers
mirror images



specific rotation → $[\alpha]_\lambda^T = \frac{\alpha}{l \times \rho}$ ← observed rotation

l ← path length

ρ ← concentration

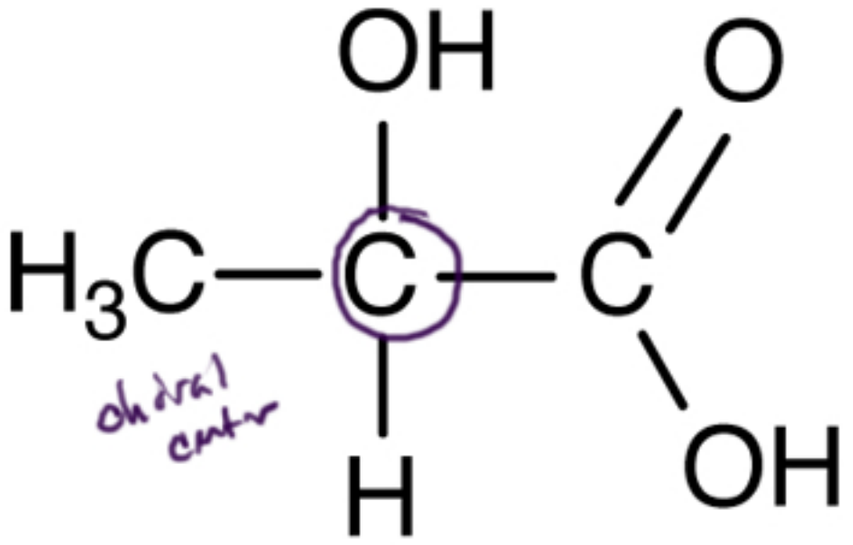
levorotatory or dextrorotatory

an optical isomer may be d or l

(THIS IS NOT THE SAME AS D and L)

polaroid filter →

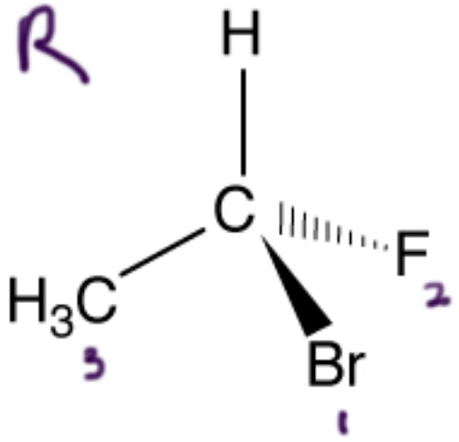
↕ plane polarized light



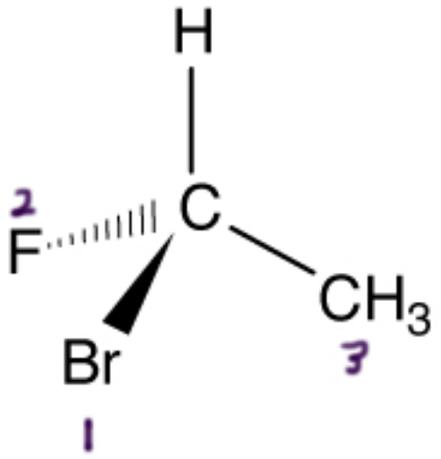
Lactic Acid

Two Enantiomers

R



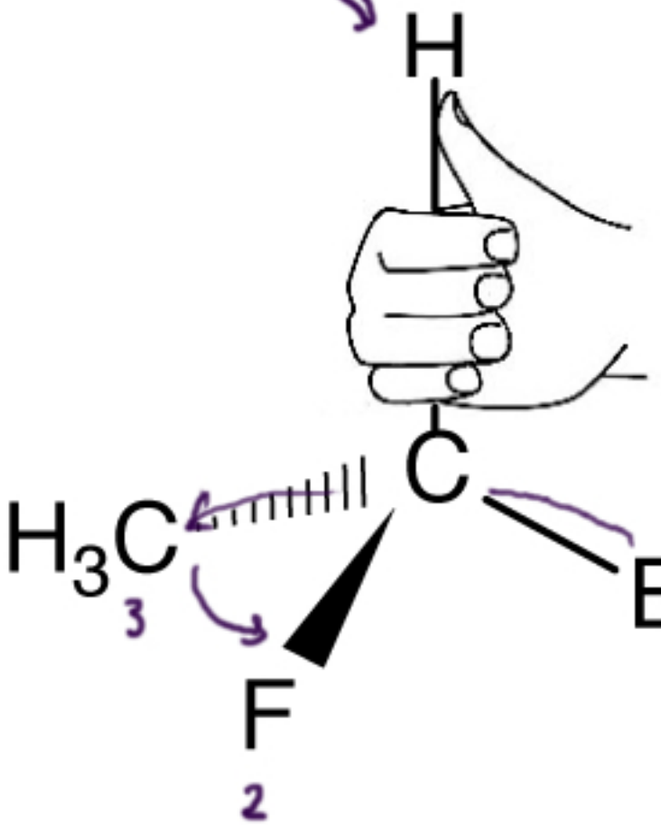
S



1 ⇒ 2 ⇒ 3

lowest rank

Cahn Ingold Prelog System



1 ⇒ 3 ⇒ 2

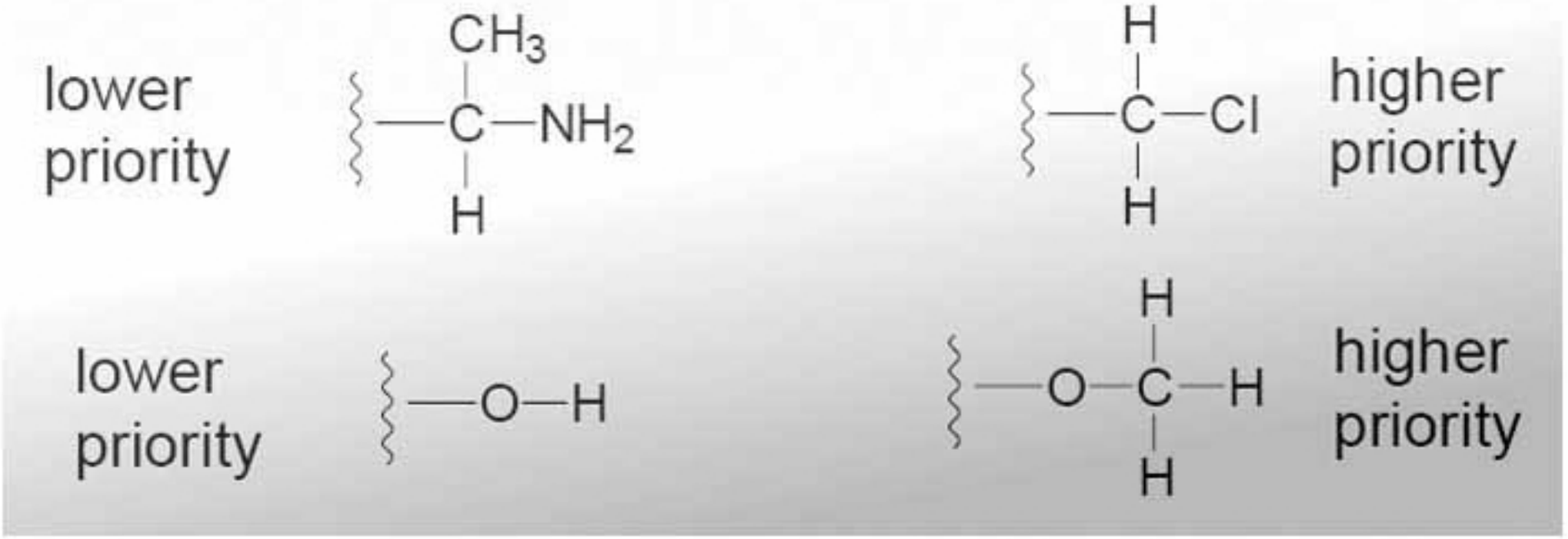
that's S

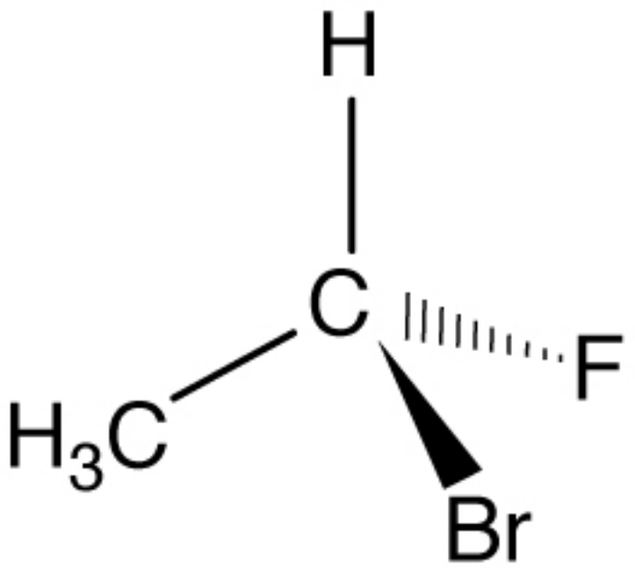
if it had been

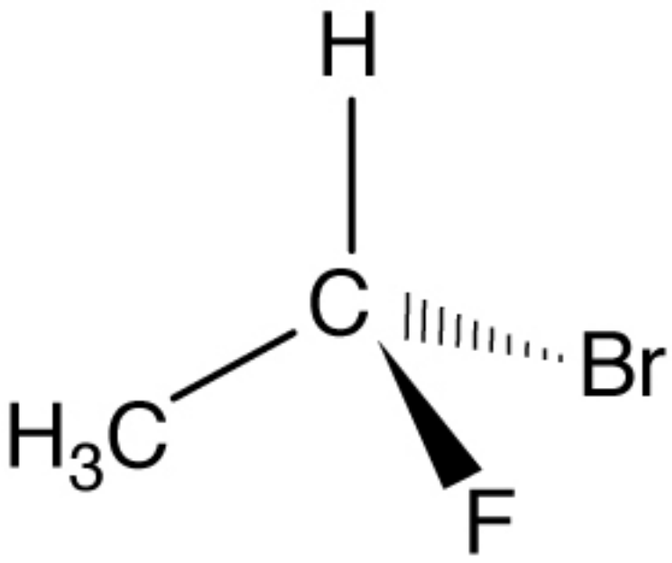
1 ⇒ 2 ⇒ 3

that's R

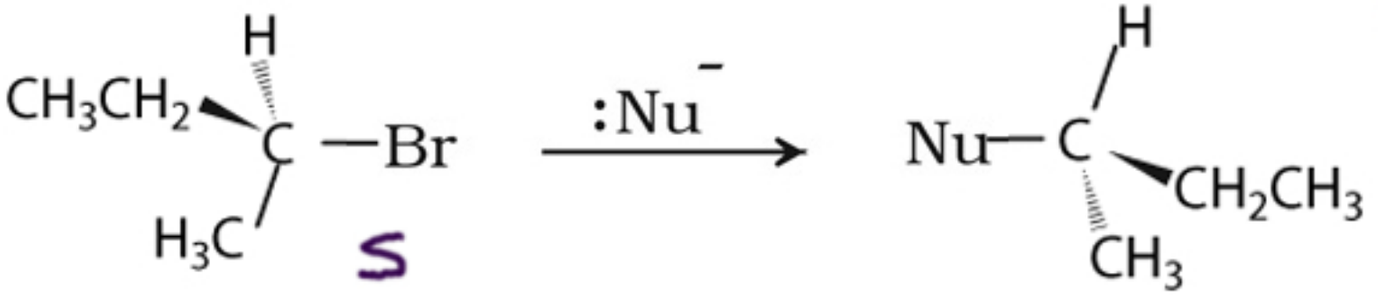
Practice!


lower priority
CH3
C
NH2
H
H
C
Cl
H
higher priority
lower priority
O
H
H
O
C
H
H
higher priority


H
C
F
H3C
Br


H
C
Br
H3C
F

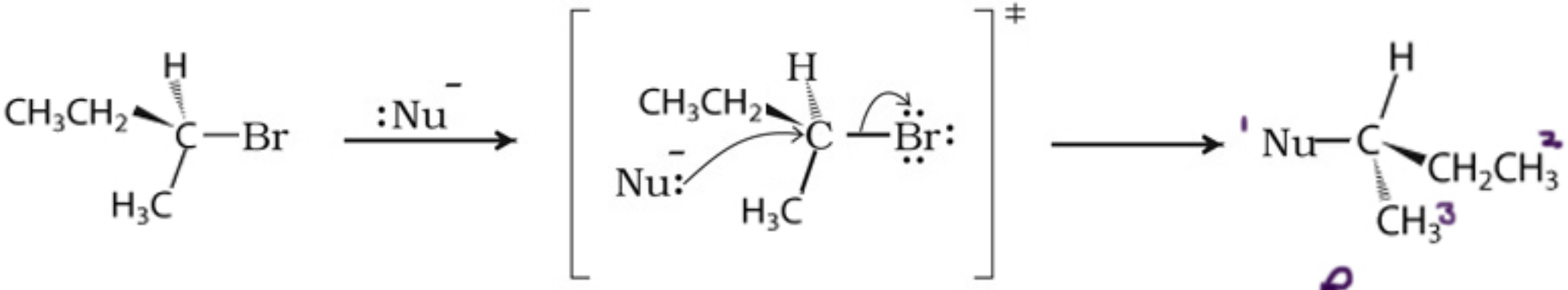
SN2



S

Alkyl halide

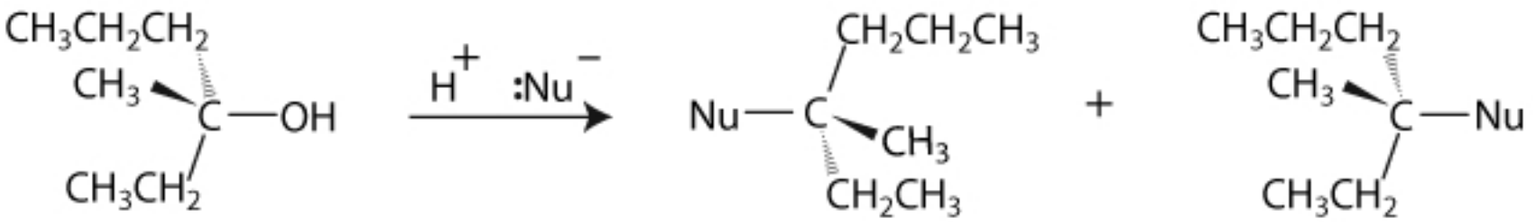
Substitution product

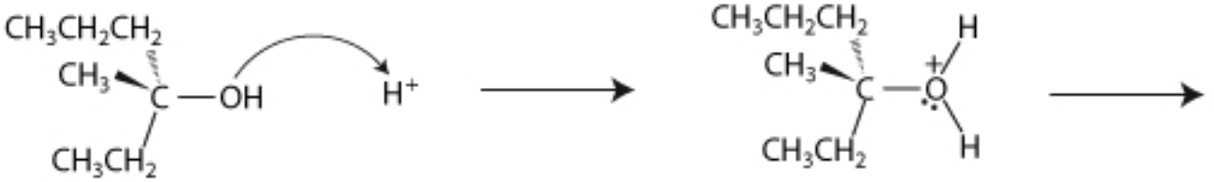


R

stereospecific for
inversion of configuration

SN1 Substitution

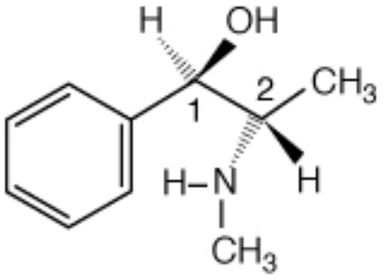




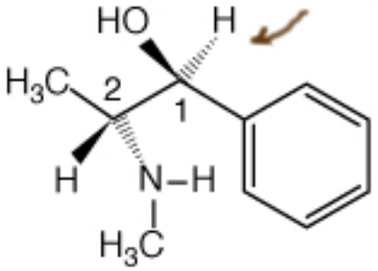
proceeds with racemization

not optically active racemic mixture

diastereomers

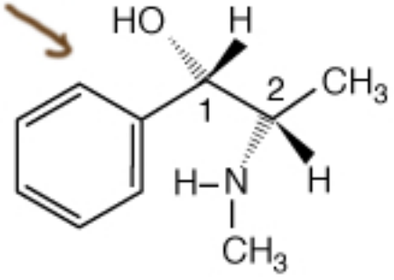


1-(*R*),2-(*S*)

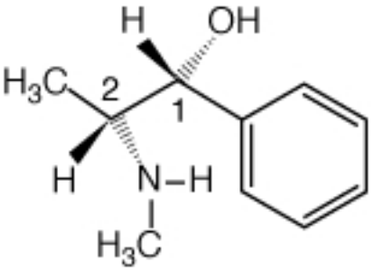


1-(*S*),2-(*R*)

Ephedrine enantiomers



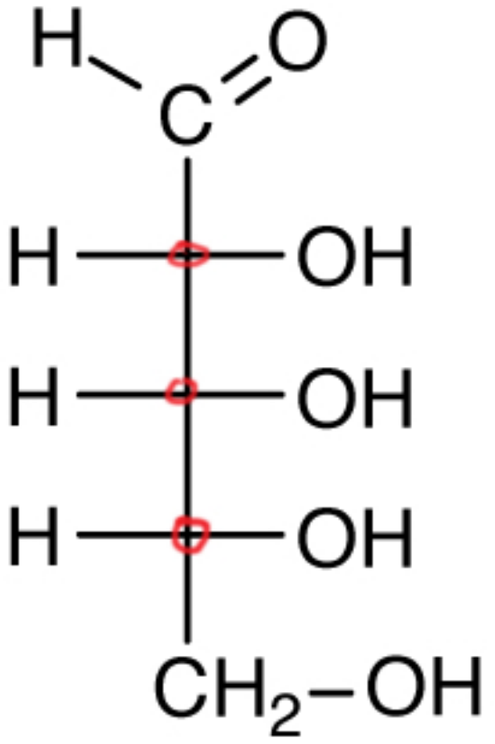
1-(*S*),2-(*S*)



1-(*R*),2-(*R*)

Pseudoephedrine enantiomers

Ribose

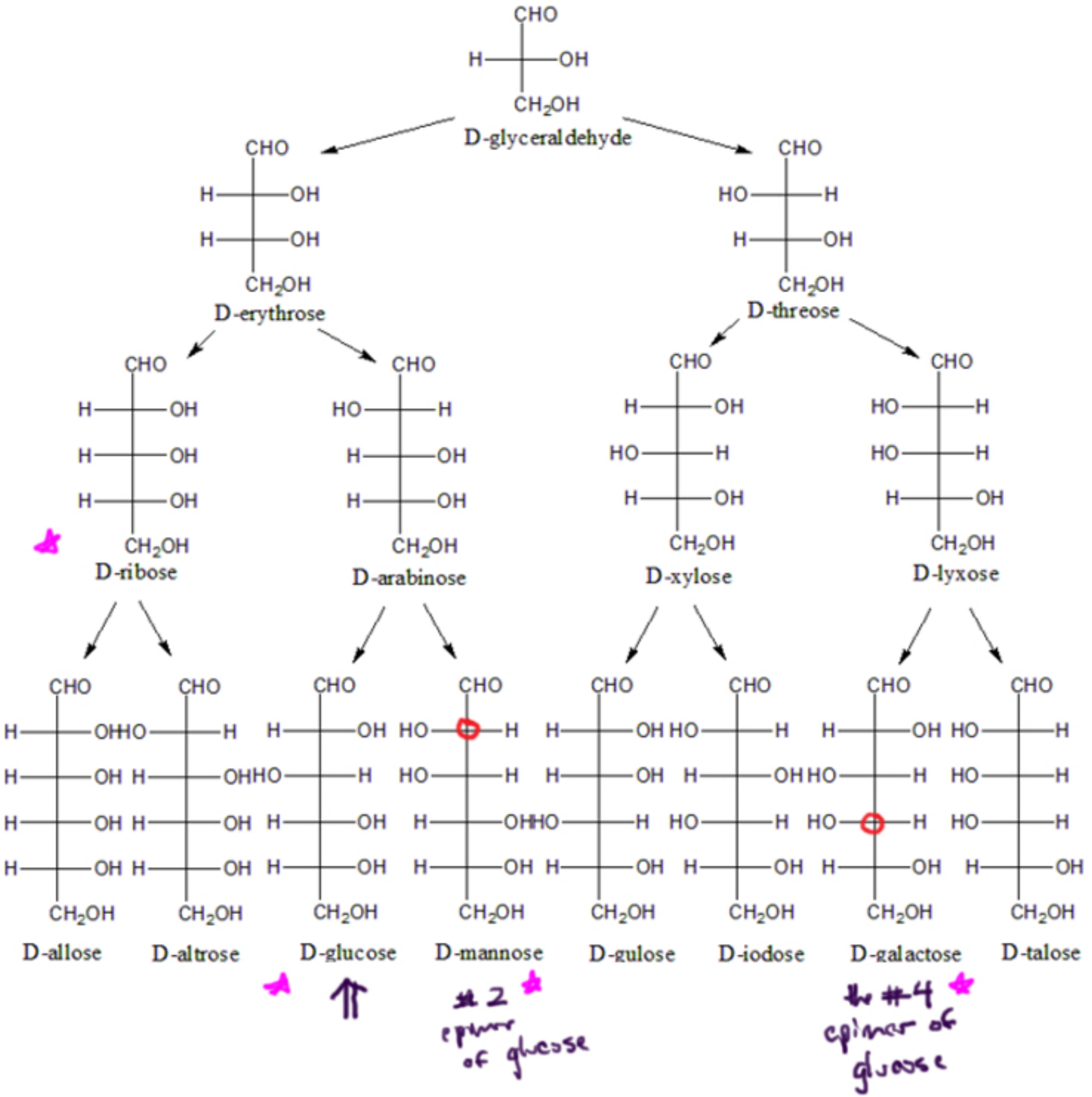


Ribose is one of

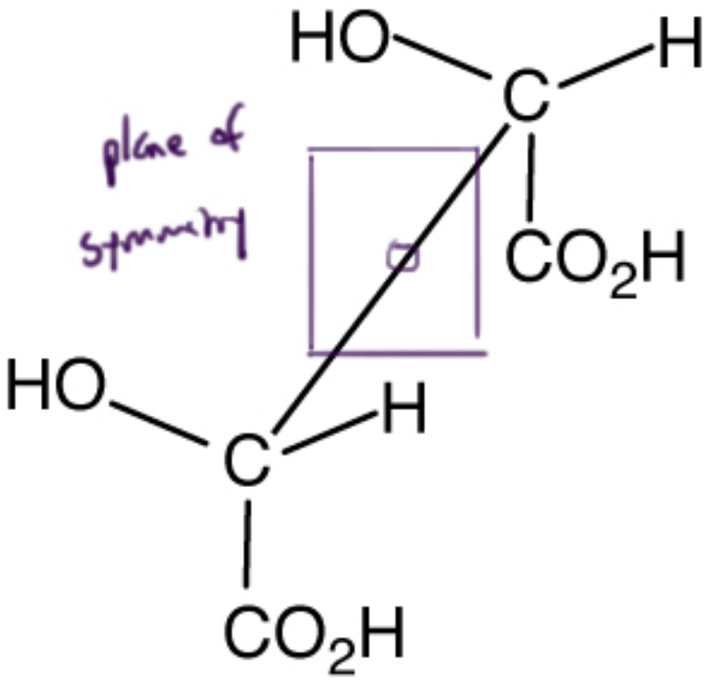
$2^3 = 8$

Stereoisomers

Fischer Projection of D- Aldoses.



Meso Compound

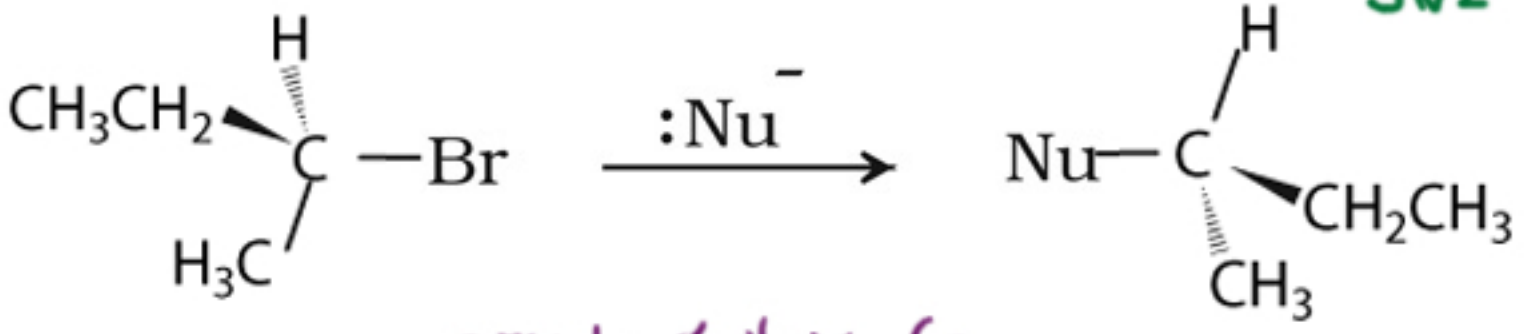


plane of symmetry

actually achiral

not optically active

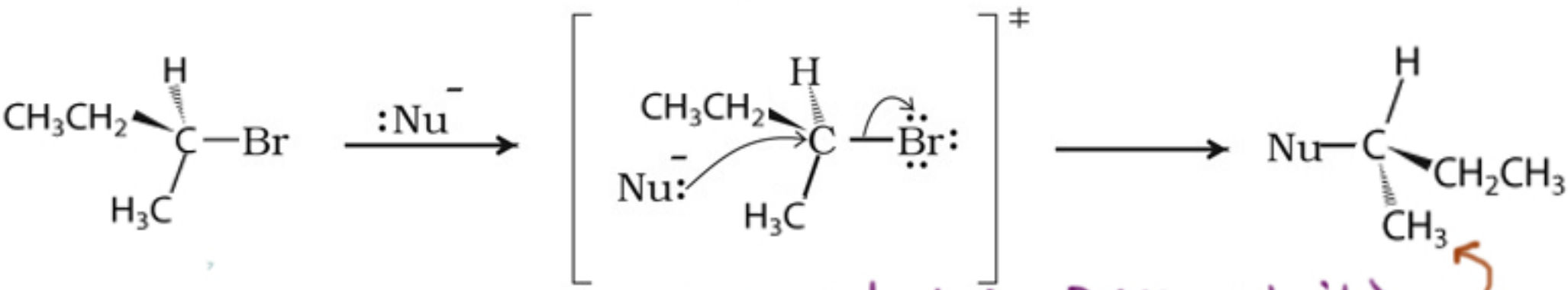
SN2 Substitution



Alkyl halide

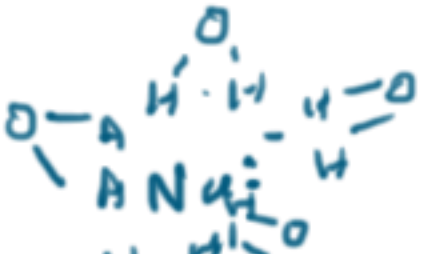
- reactor of choice for primary alkyl halides
- prefers unhindered substrate and nucleophile
- unless strong, bulky, hindered base - for 1°, tert-butoxide then E2 elimination

Substitution product



- polar aprotic solvent like DMSO, acetonitrile

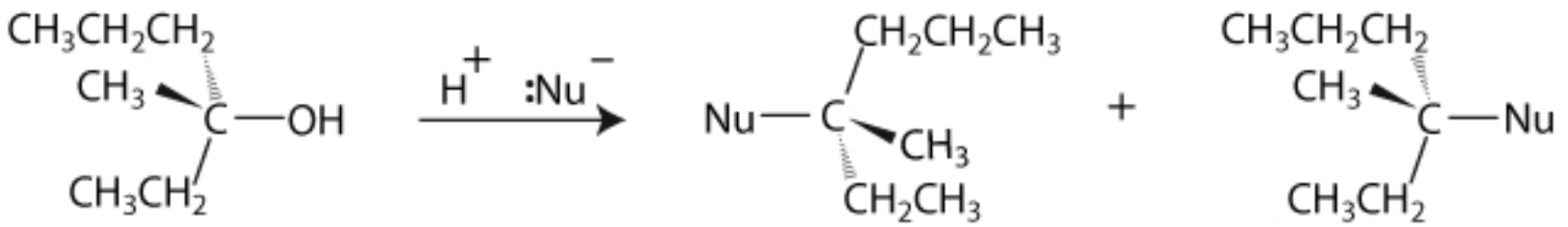
stereospecific for inversion of configuration

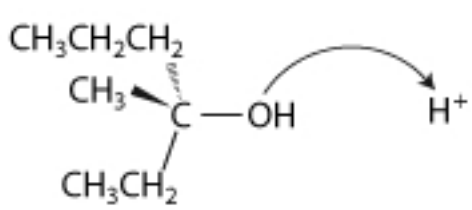


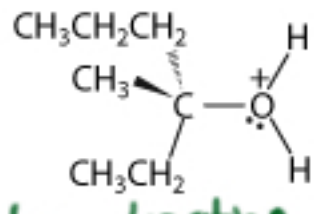
Why is a protic solvent a bad idea? Destabilizes the nucleophile.

$$\text{rate} = k\,[Nu][RX]$$

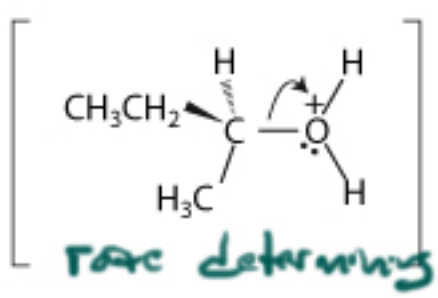
SN1 Substitution





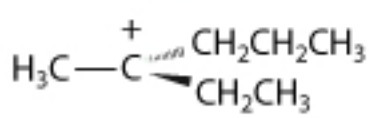


electron donating by induction

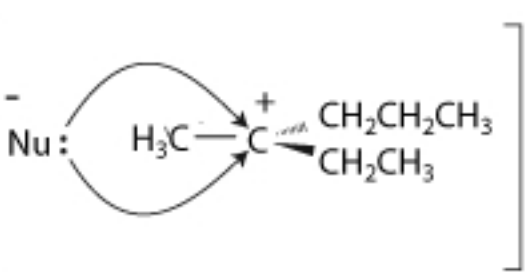


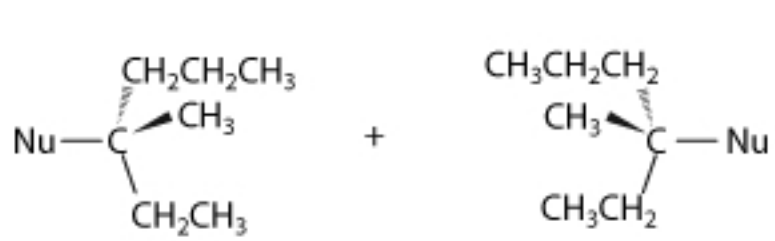
rate determining

$3° > 2° > \cancel{1°}$



carbocations might rearrange

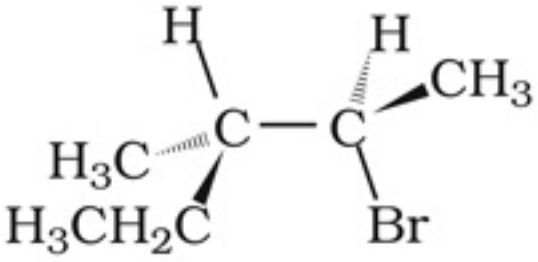




racemic mixture

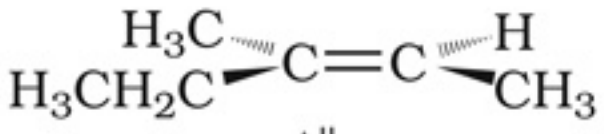
$\text{rate} = k[RX]$

E2 Elimination



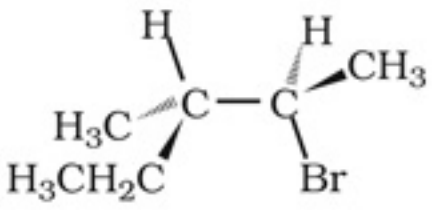
Alkyl halide

:Base⁻ →

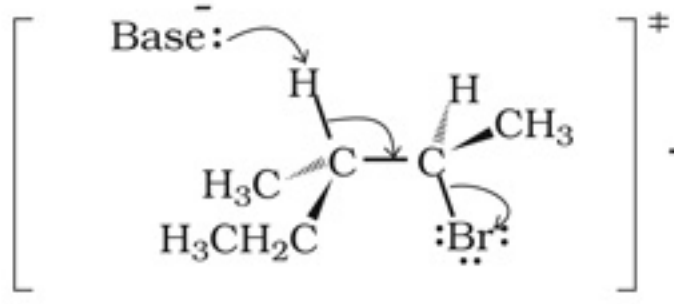


Alkene

- With 1° substrate - E2 occurs with a bulky hindered base
- with 2° - strong bases



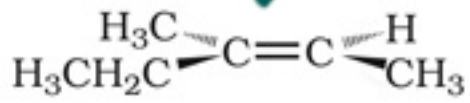
:Base⁻ →



anti periplanar transition state

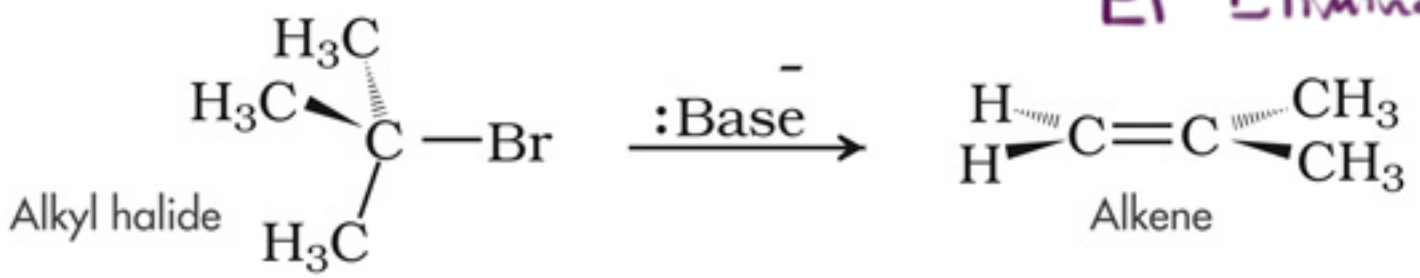
→

more substituted double bond is favored Zaitsev's rule



In this case the reaction is stereospecific for cis. (anti-periplanar transition state)

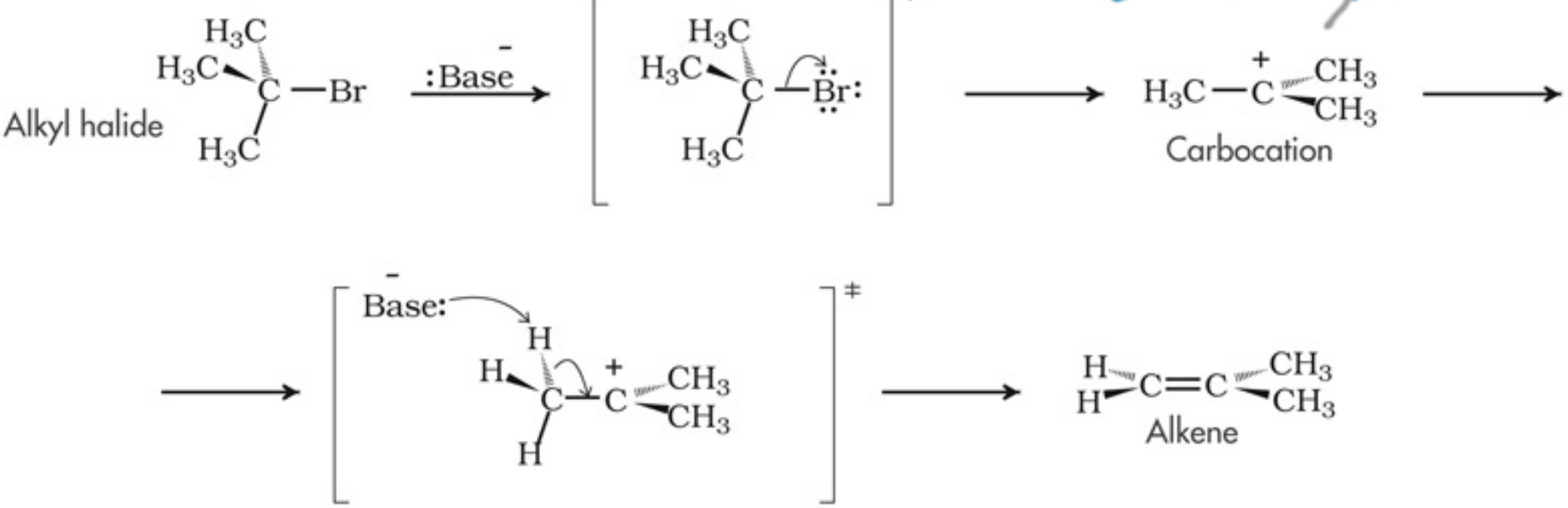
E1 Elimination



Alkyl halide

Alkene

3° > 2° > 1°

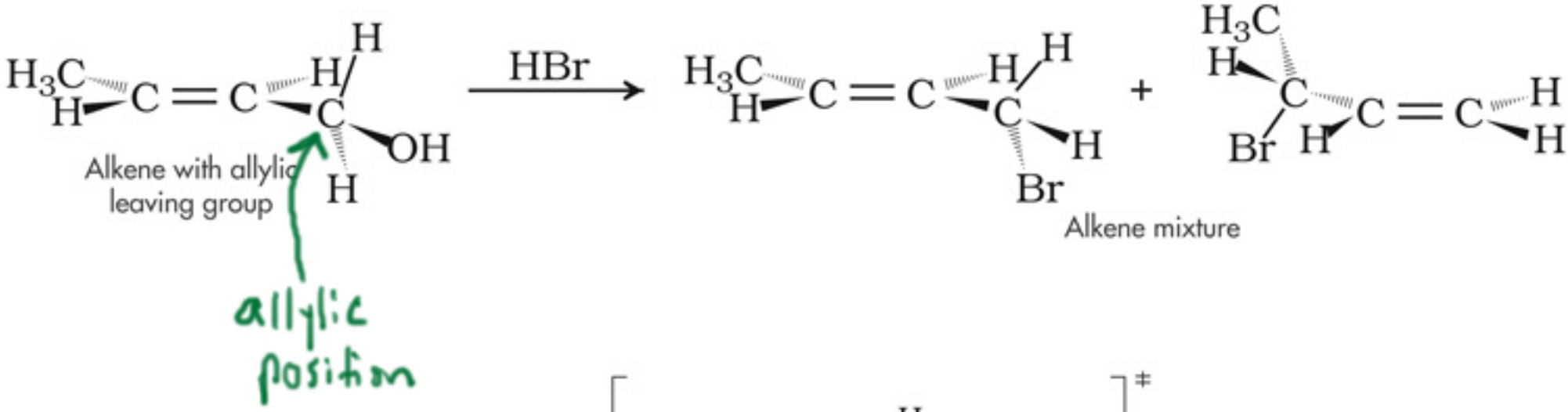


Alkyl halide

Carbocation

Alkene

Often in mixture with SN1


Alkene with allylic leaving group
HBr
Br
Alkene mixture
allylic position
Alkene with allylic leaving group
HBr
Oxonium ion
allylic > 3° > 2° > 1°
Allylic carbocation intermediate
benzylic
Br
Alkene mixture

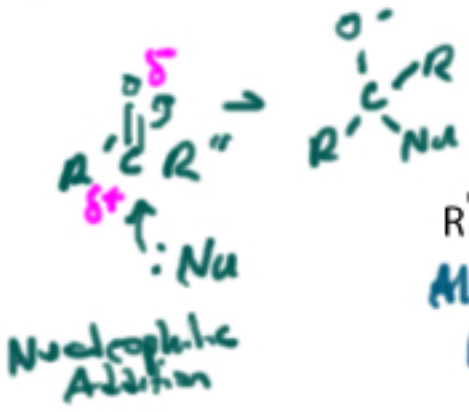
Substrate	If the substrate is a primary alkyl halide, the reaction will almost certainly be SN2. Exceptions: A bulky hindered base like tert-butoxide will tend to react with E2. Watch out for allylic primary alkyl halides. If the substrate is tertiary, the reaction cannot be SN2.

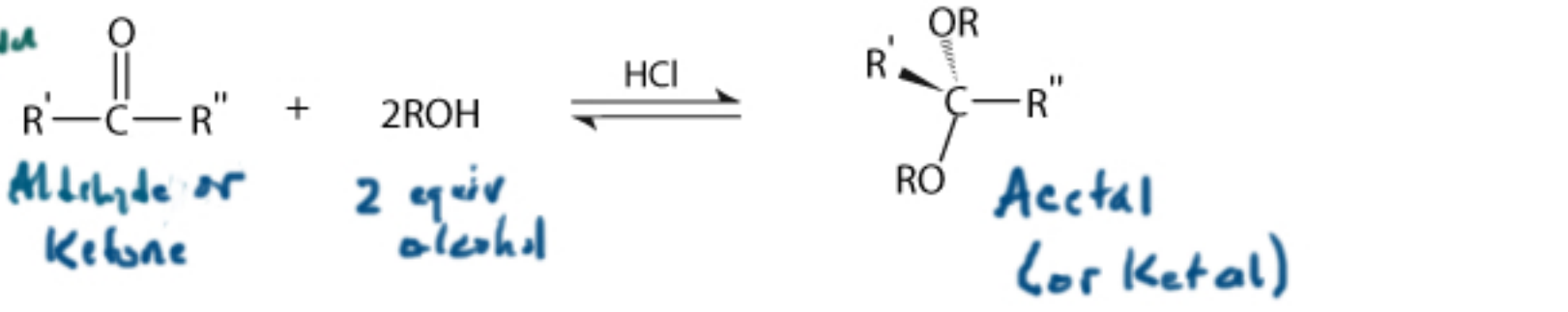
Nucleophile	Charged nucleophiles/bases will favor SN2/E2. Deciding between SN2 & E2, look at the basicity. Strong bases with secondary subtrates will favor E2. Weak bases like Cl-, CN- favor SN2. Uncharged nucleophiles/bases favor SN1/E1.

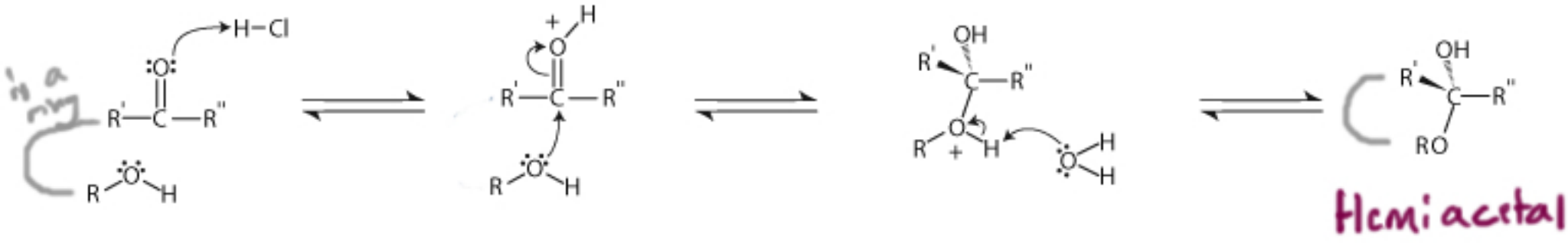
Solvent	SN2 substitution is favored by polar, aprotic solvents like DMSO, acetonitrile, diethyl ether etc.

Temperature	If the choice is between E1 and SN1, high temperature favors elimination.

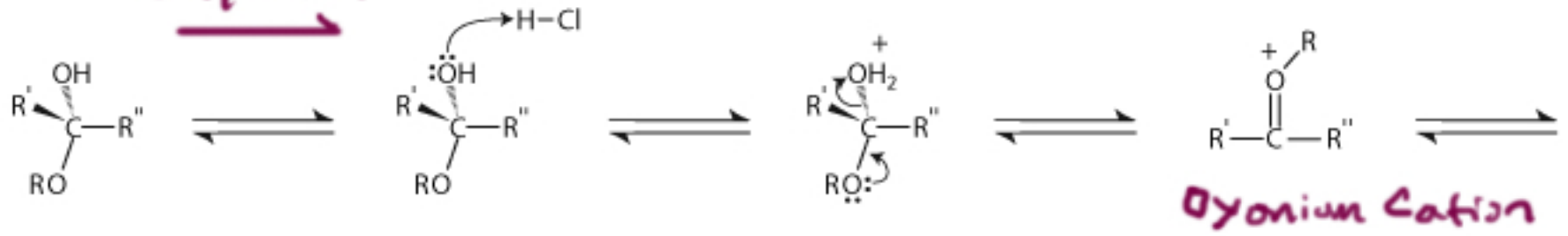
Acetal Formation

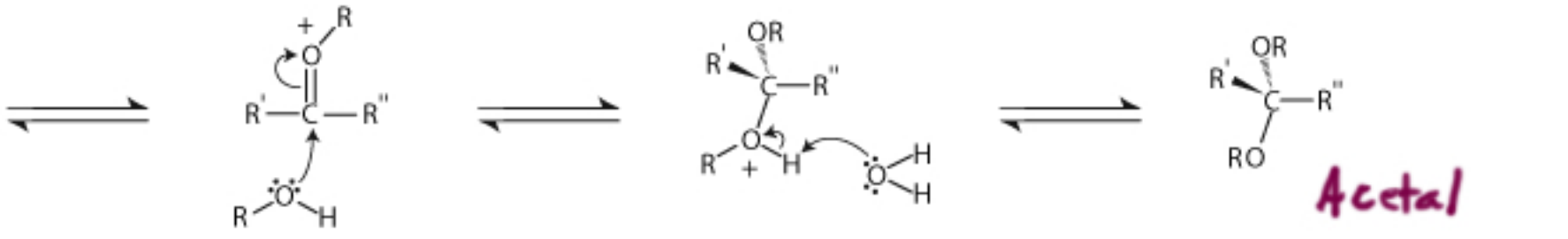






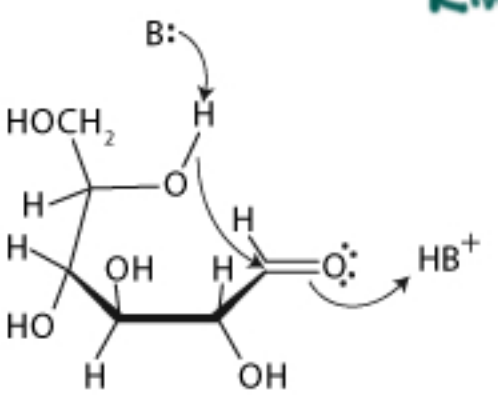
Dehydration →

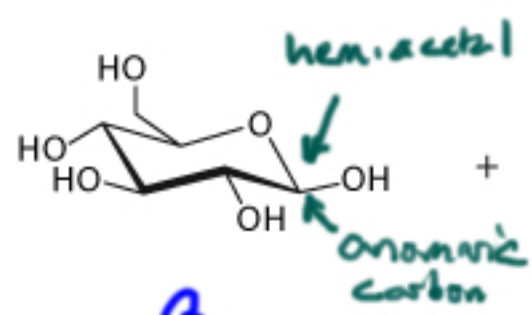




Benchtop - used to protect carbonyl groups

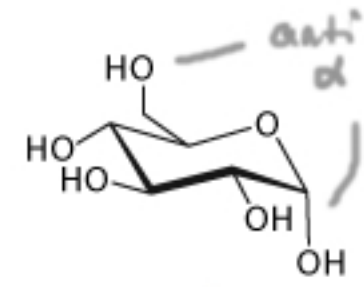
Ring Formation in Glucose (Hemiacetal Formation)





β

≈ 65%

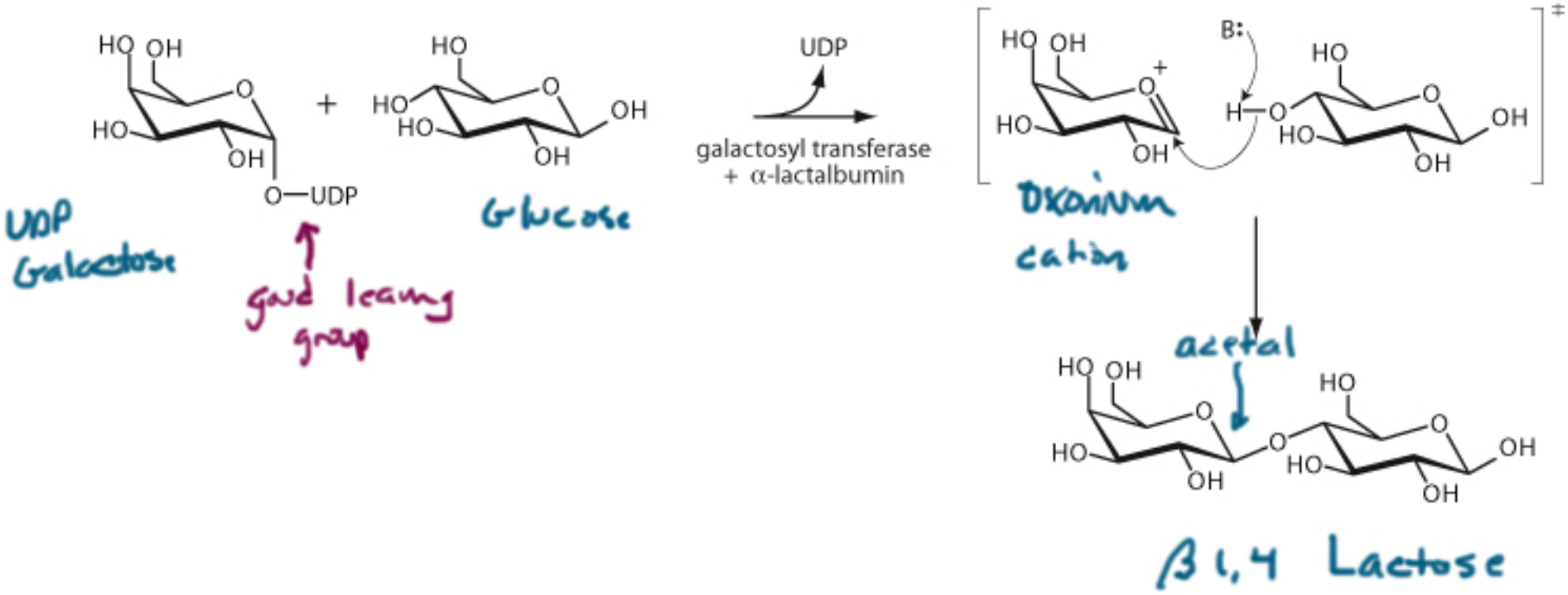


α

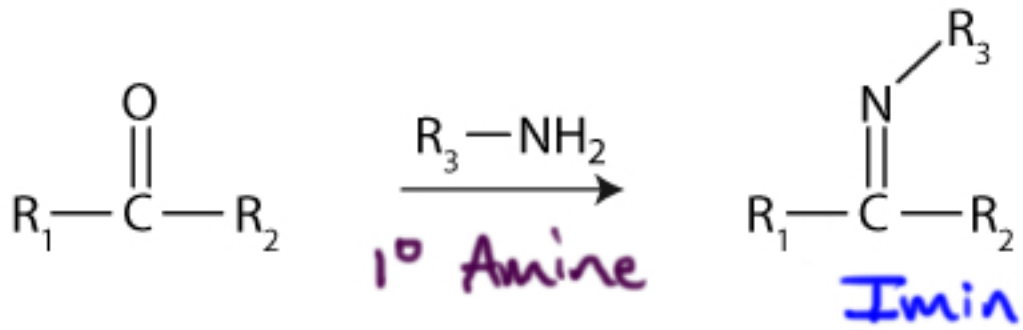
≈ 33%

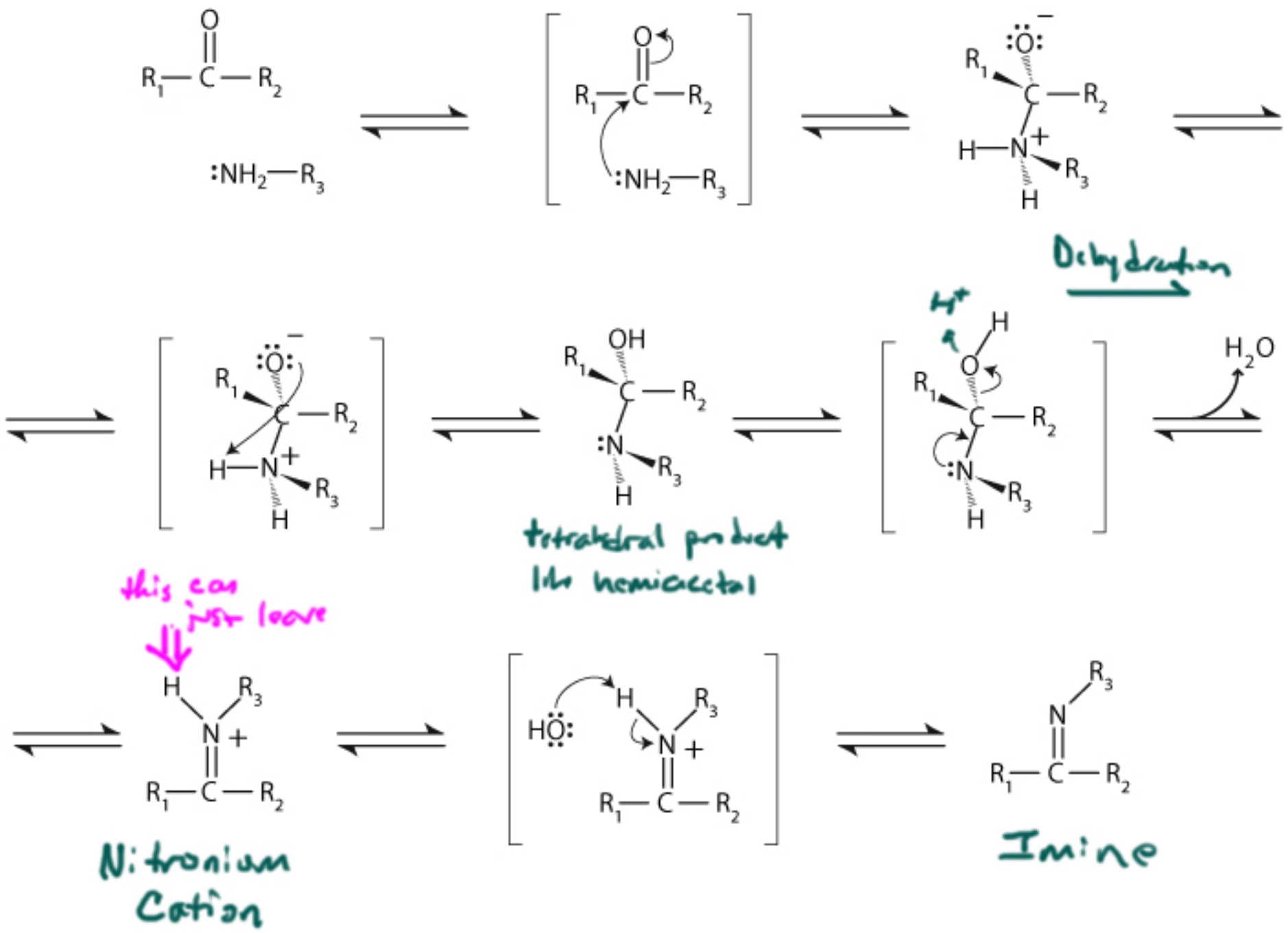
2 anomers of D-glucopyranose

Forming a Glycosidic Bond (bit step 2 of acetal formation)

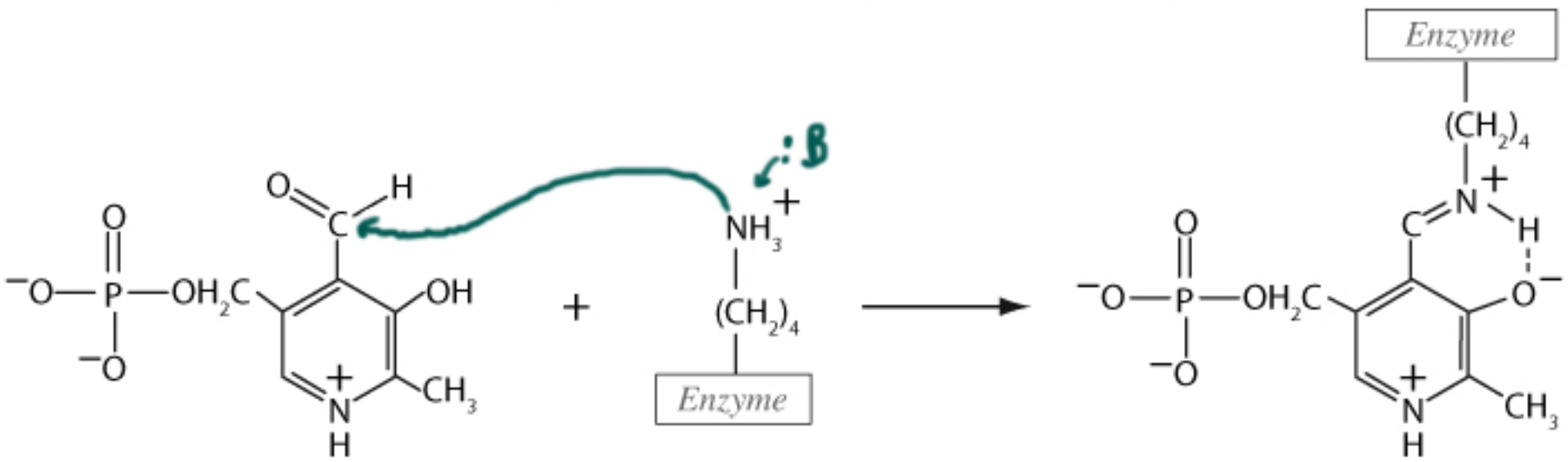


Imine Formation



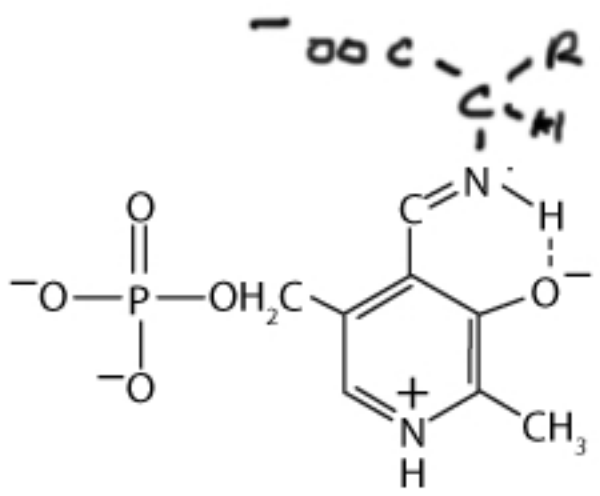


Formation of Enzyme PLP Schiff Base



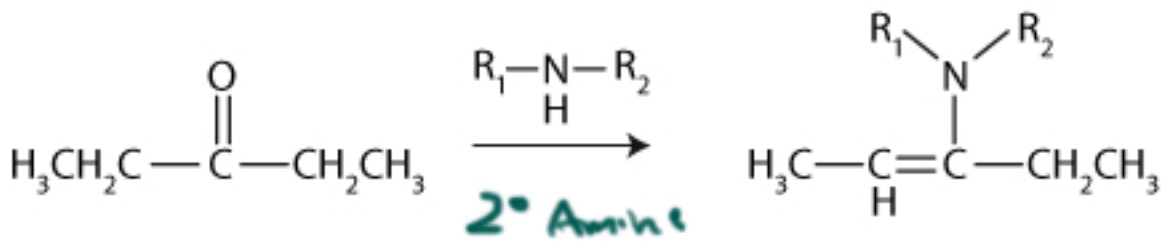
PLP

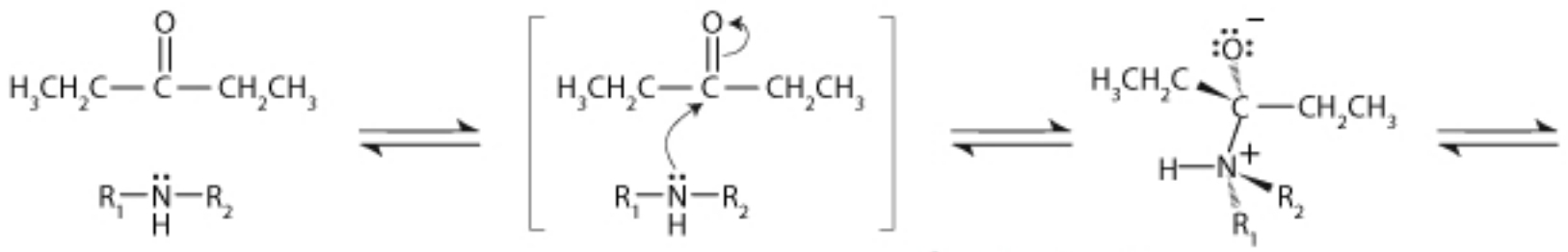
"the amino acid cofactor"

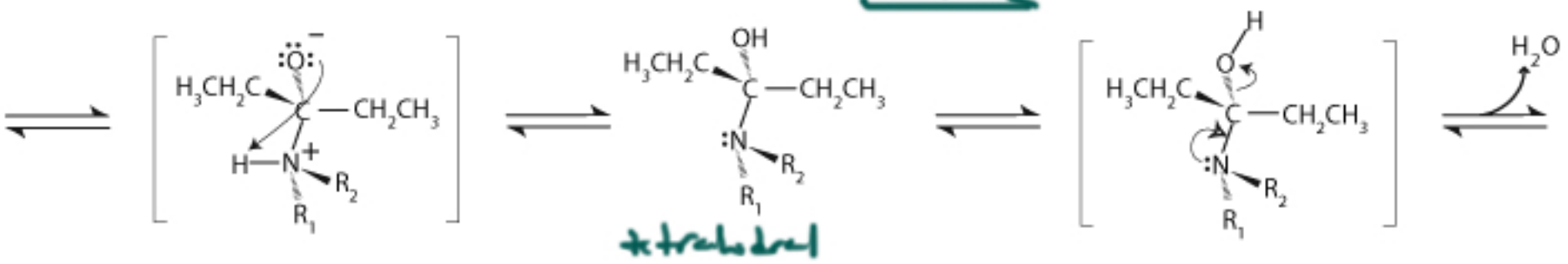


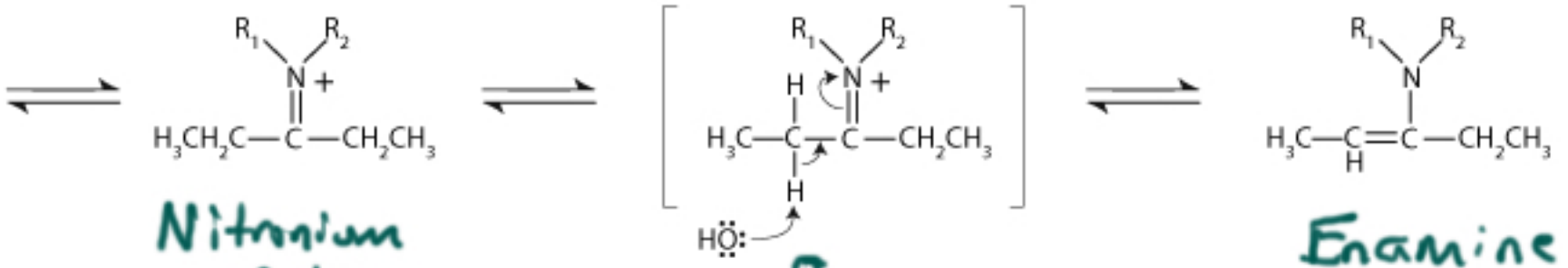
amino acid PLP Schiff base

Enamine Formation



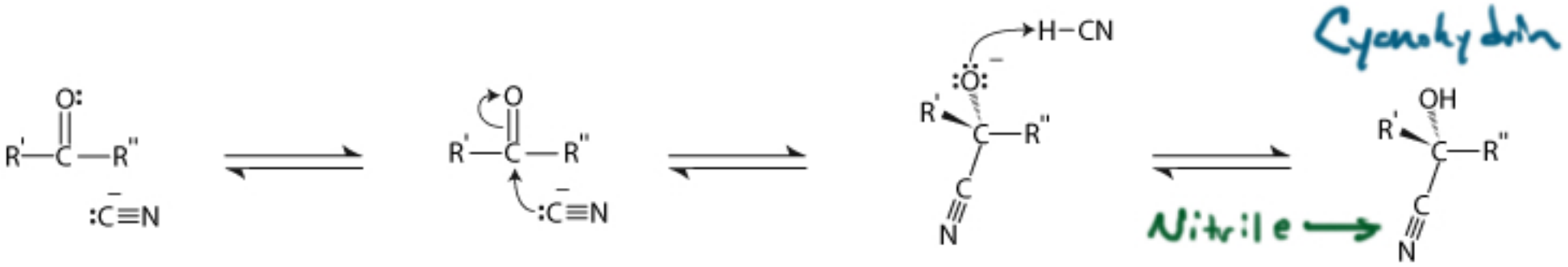






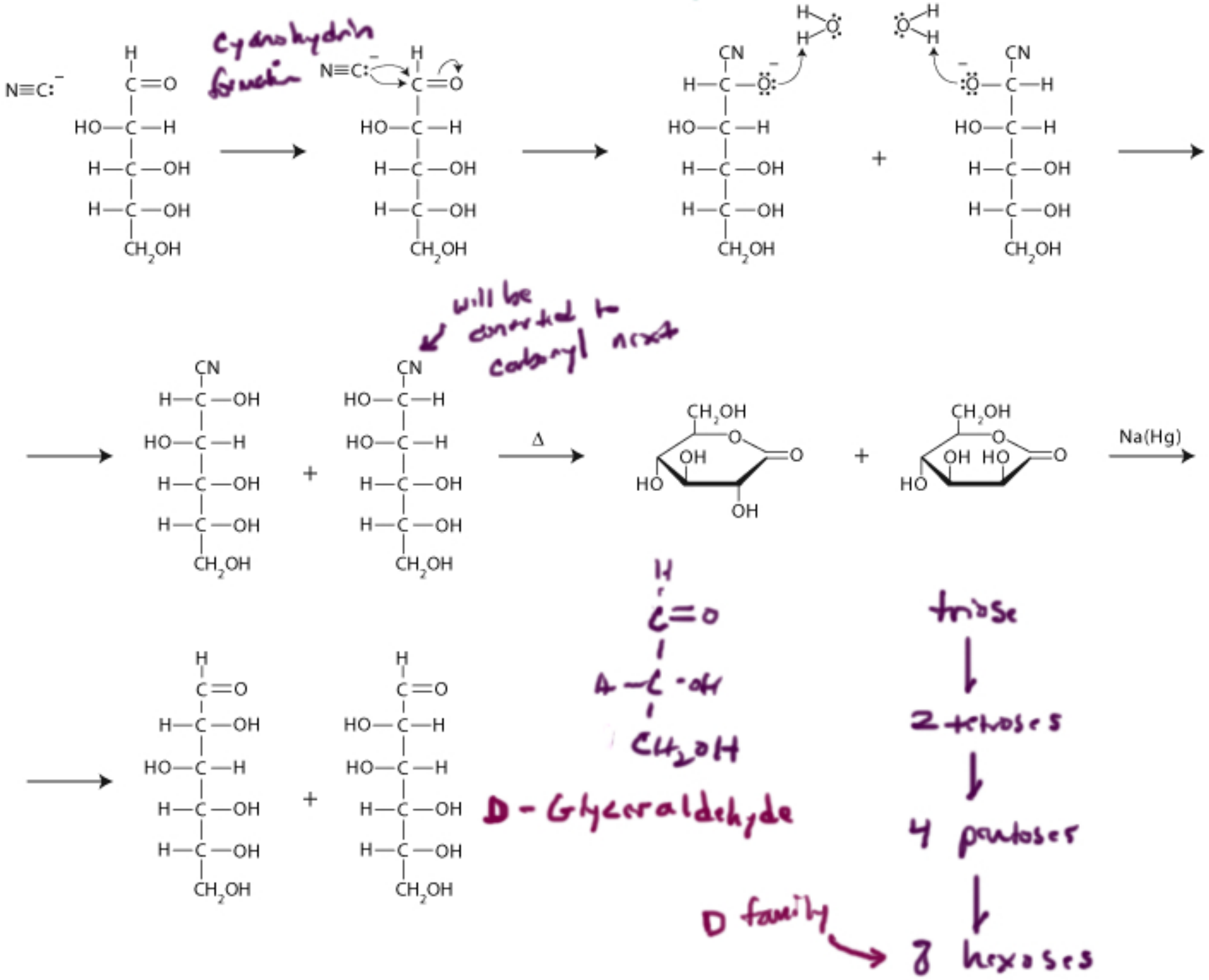
Transfer of an α hydrogen

Cyanohydrin Formation



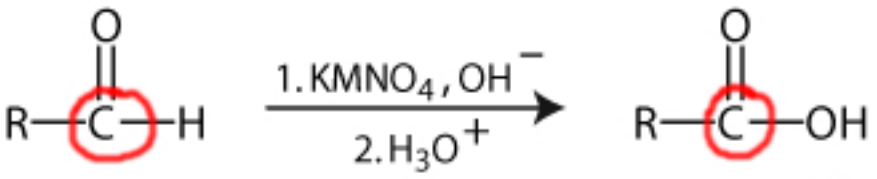
Hydrolysis of Nitrile | $2 H_2O$ (or OH^-)

Kiliani Fischer Synthesis



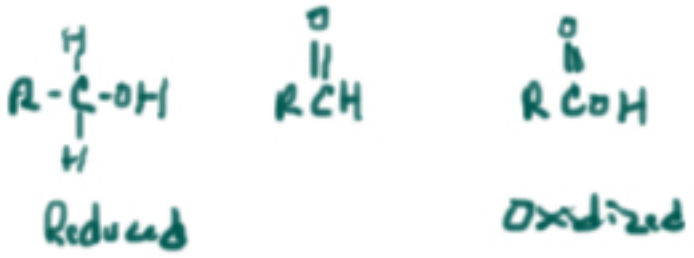
Steps of the Kiliani-Fischer synthesis of D-glucose and its C-2 epimer, D-mannose, from D-arabinose

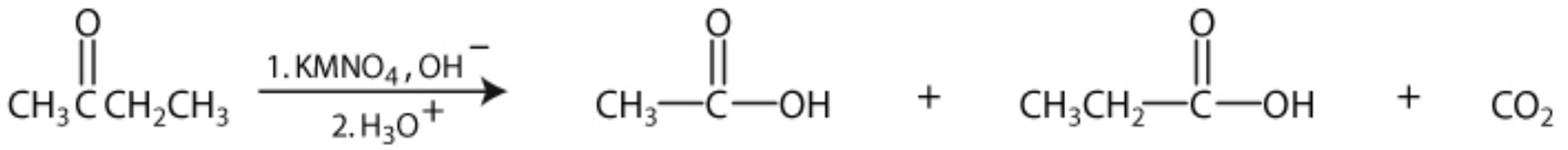
Oxidation of Aldehydes and Ketones



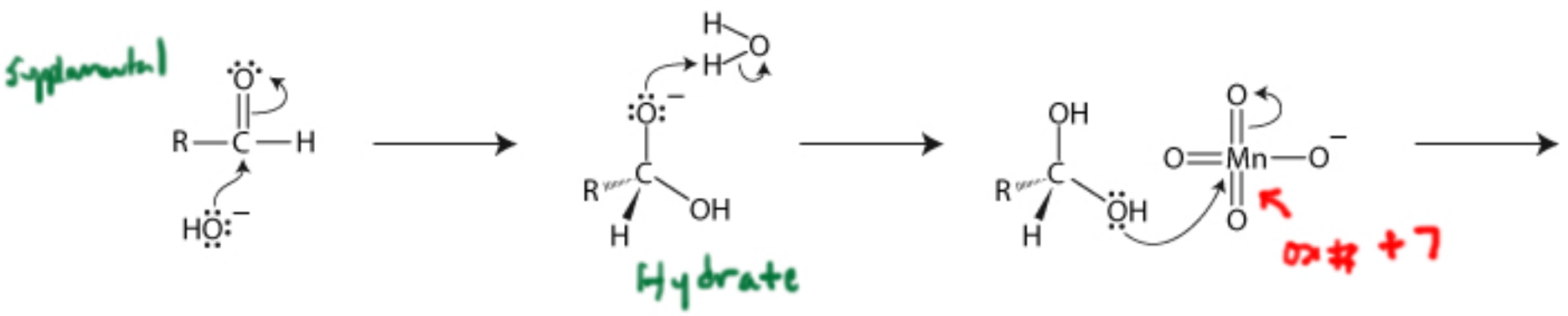
ox # +1

ox # +3

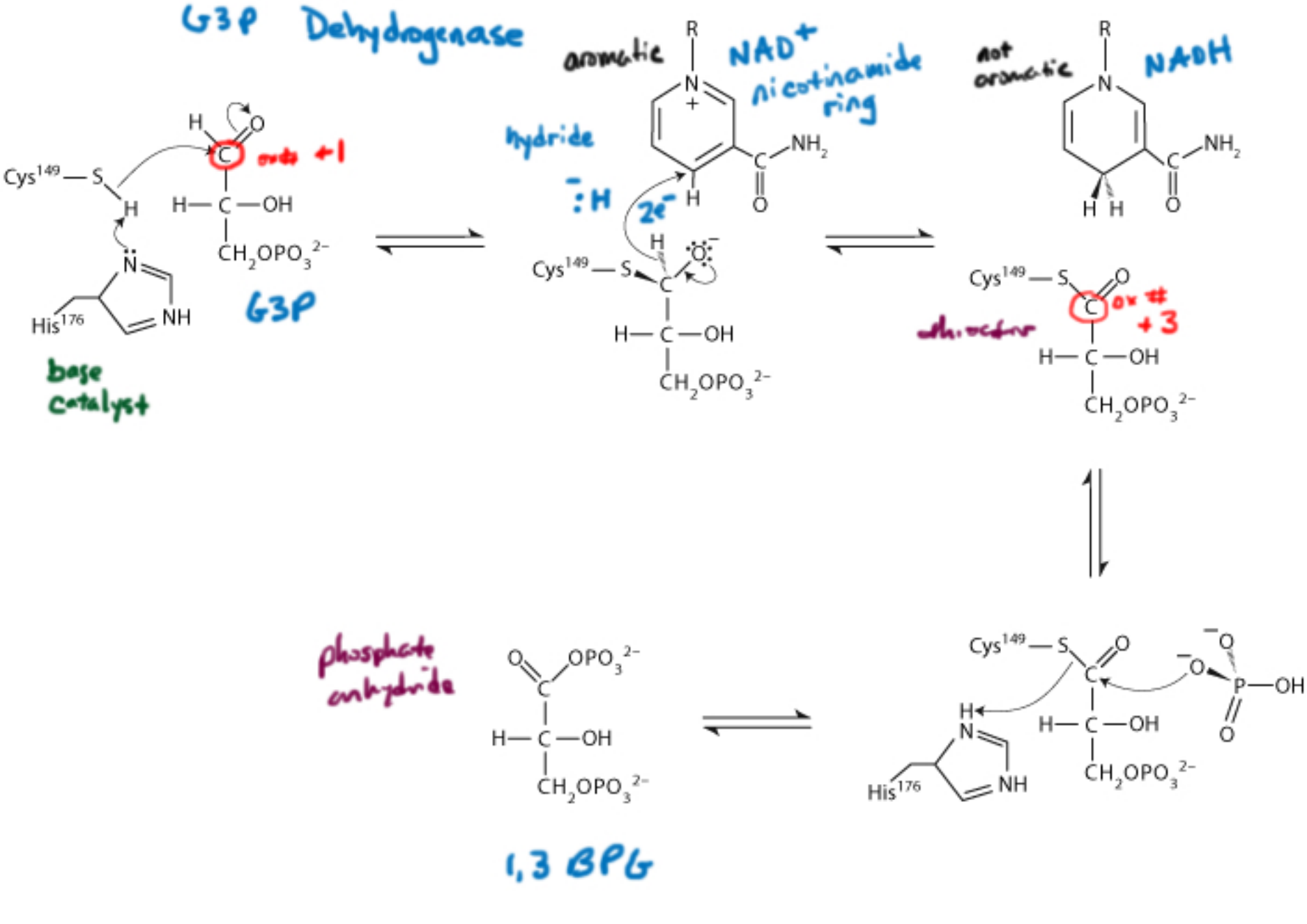




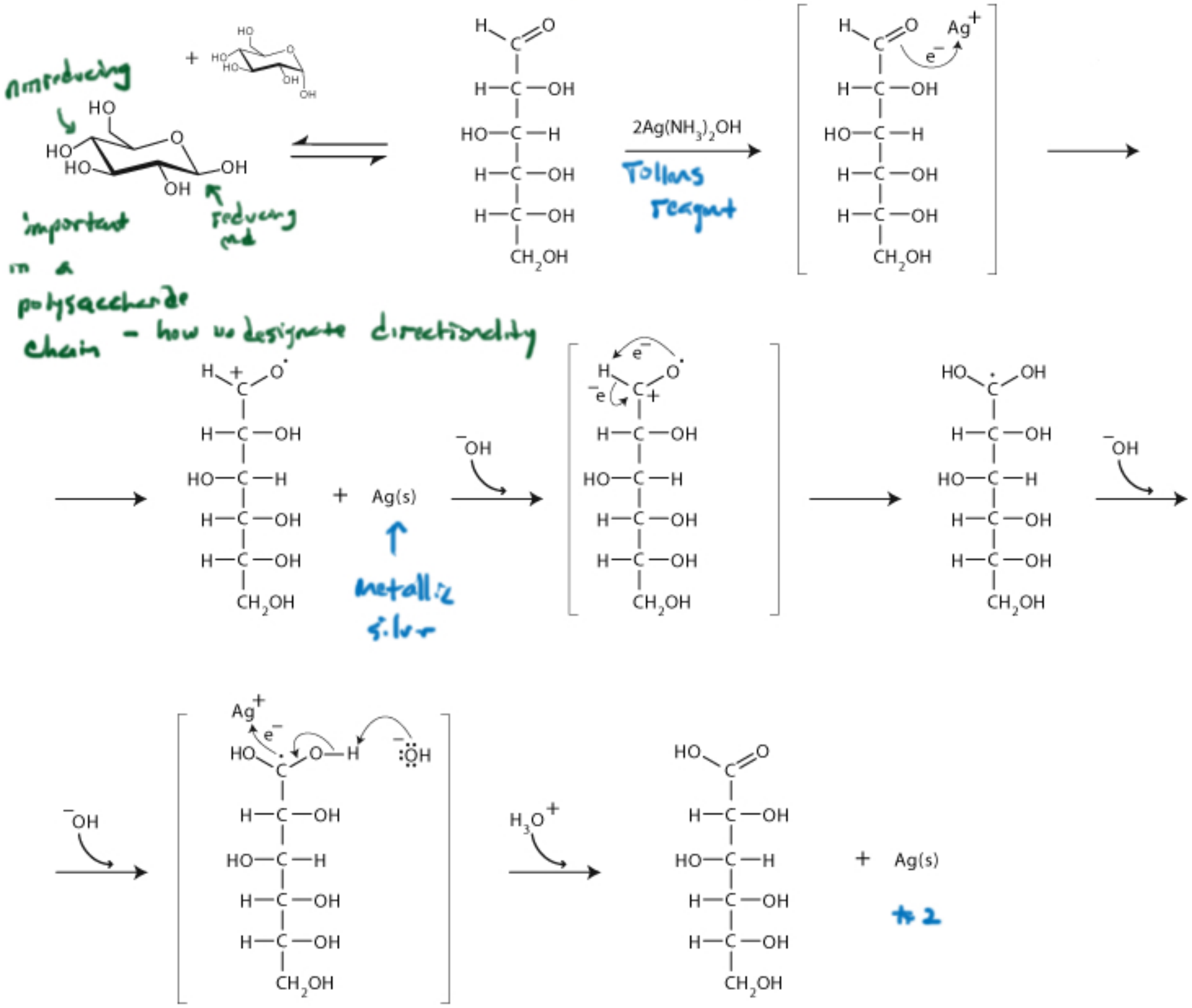
symmetrical



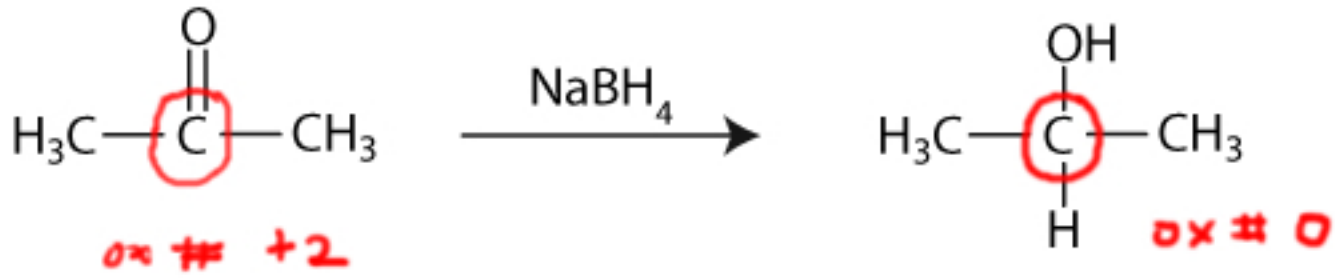
G3P Dehydrogenase

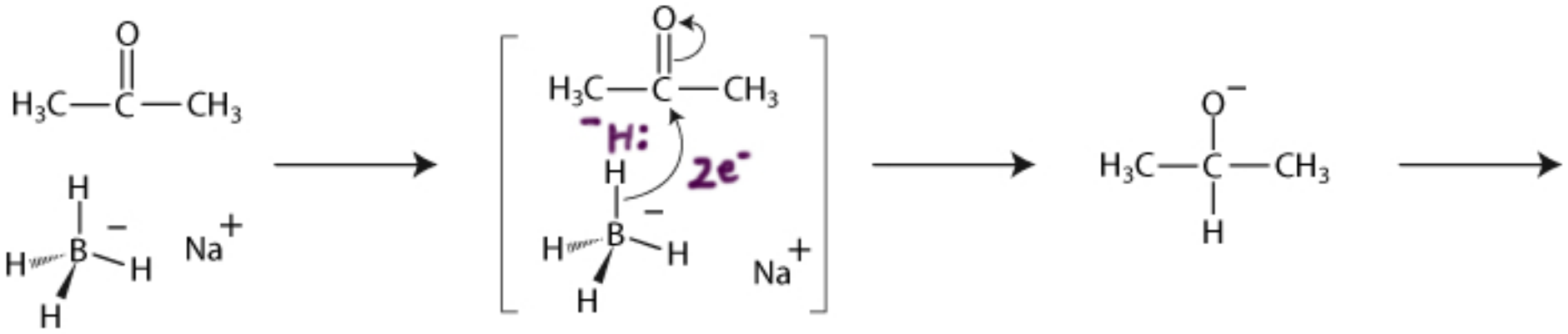


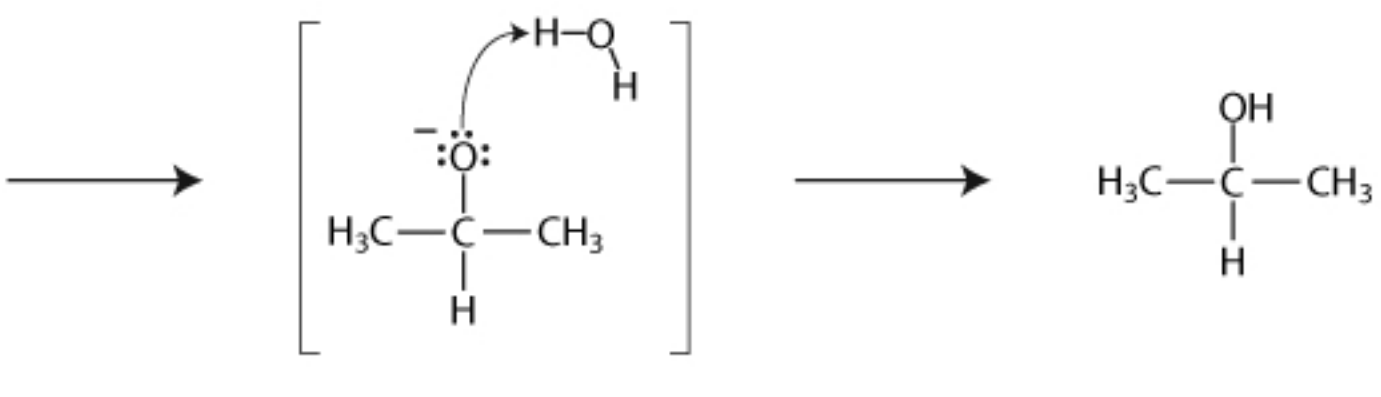
Tollens Test for reducing sugars



Reduction of Aldehydes and Ketones

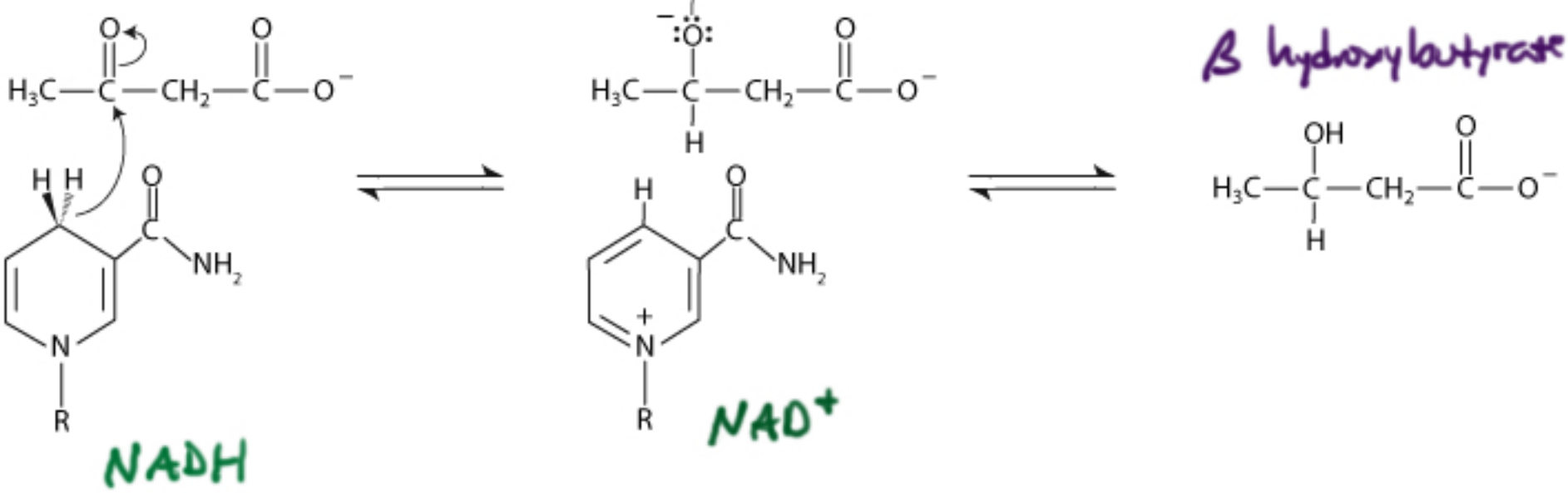






β Hydroxybutyrate Dehydrogenase

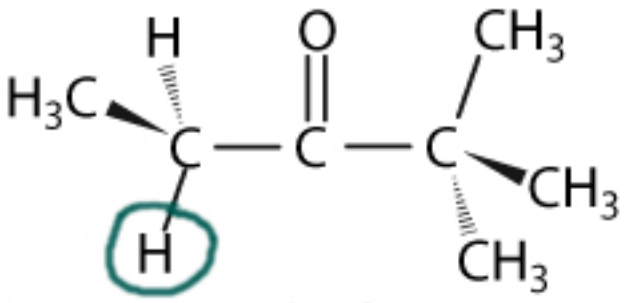
Acetoacetate



Acetoacetate and β hydroxybutyrate are ketone bodies

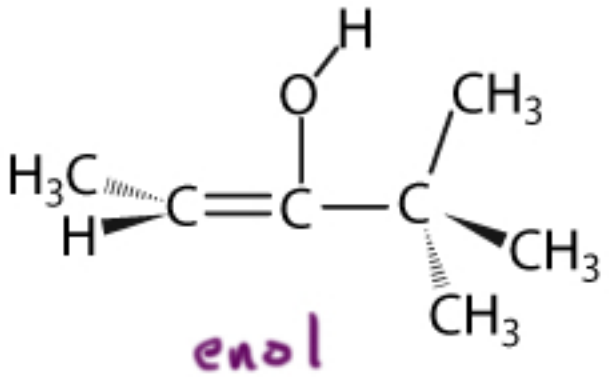
Tautomers - Constitutional isomers that interconvert

Keto Enol Tautomerism

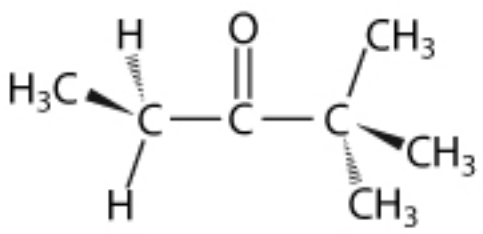


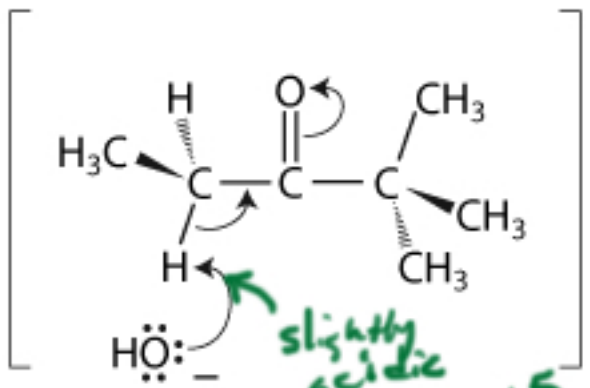
α hydrogen

aldehyde or ketone with α hydrogens



enol



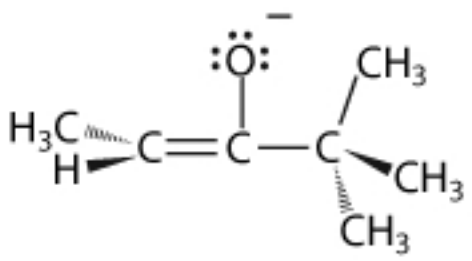


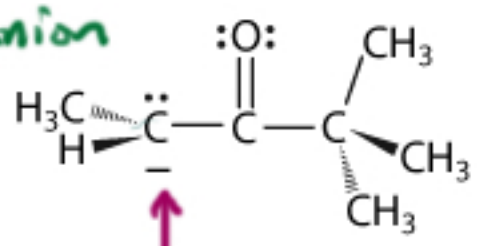
slightly acidic pKa ~ 15

$HA \rightleftharpoons A^- + H^+$

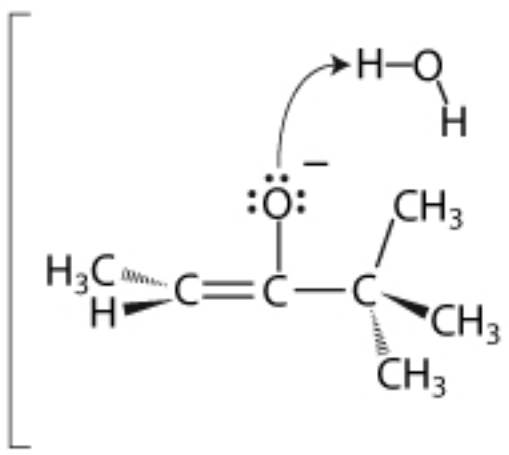
$K = e^{-\Delta G^\circ / RT}$

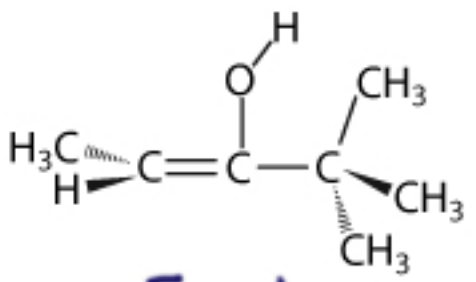
resonance stabilized enolate anion





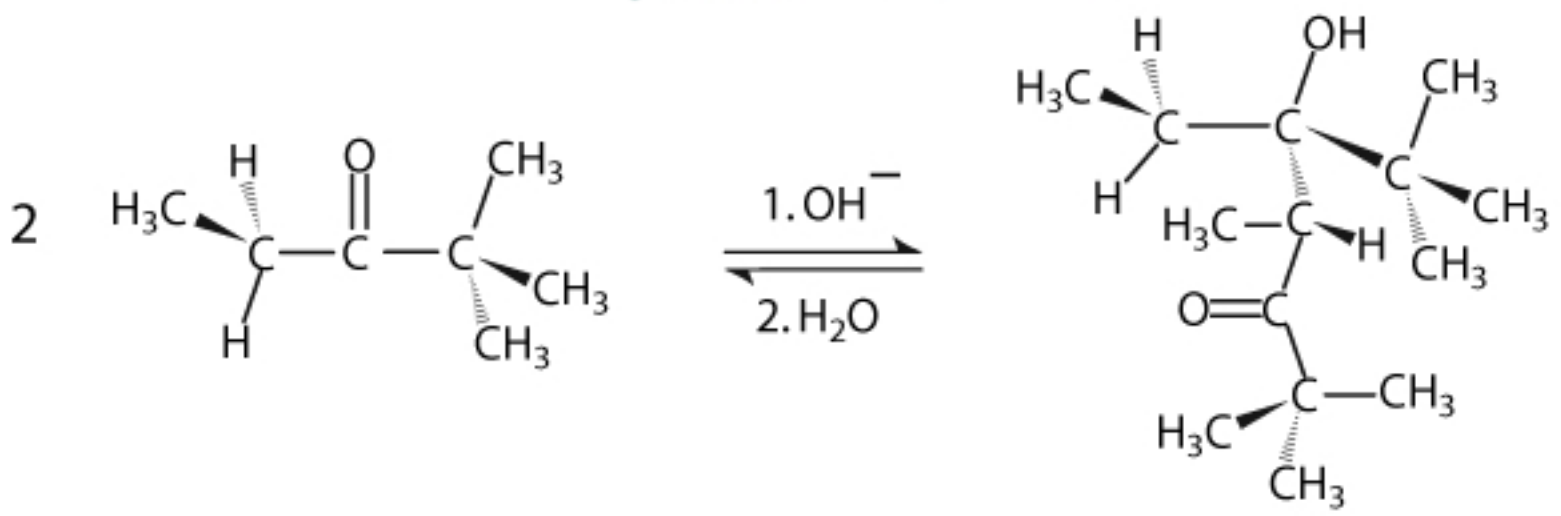
nucleophilic

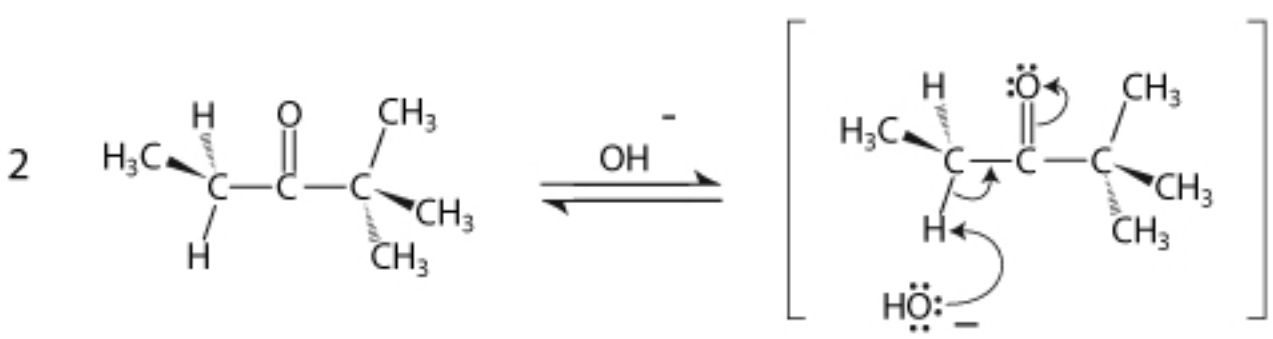




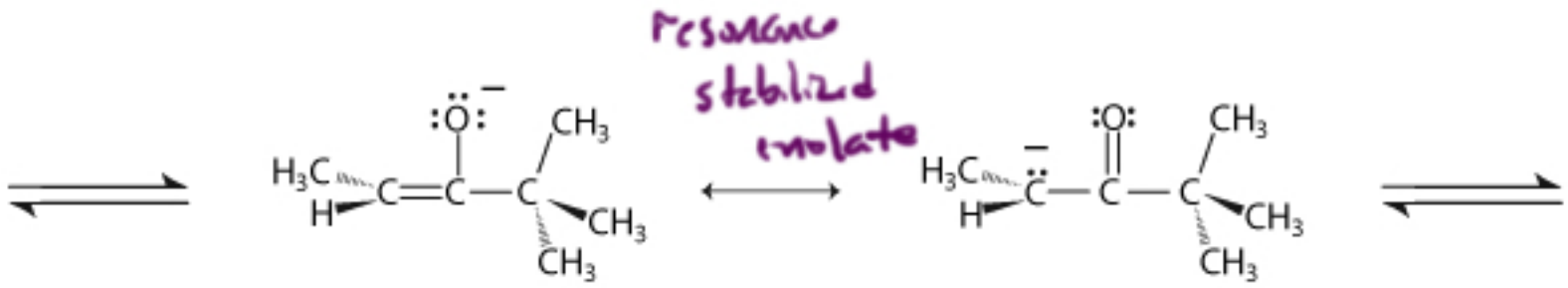
Enol

Aldol Addition

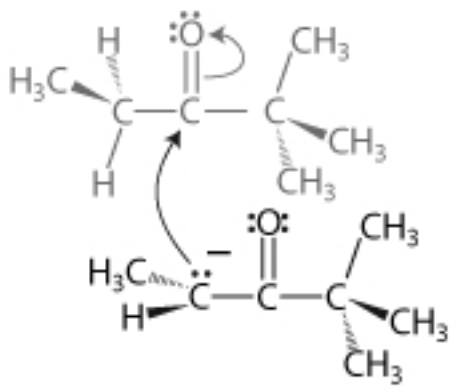


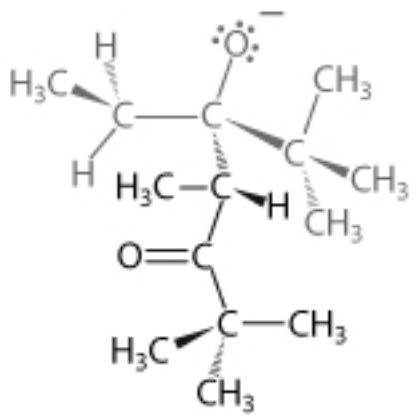


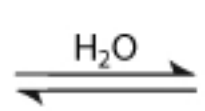
Base catalyzed enolate formation



the enolate of one attacking the carbonyl of another

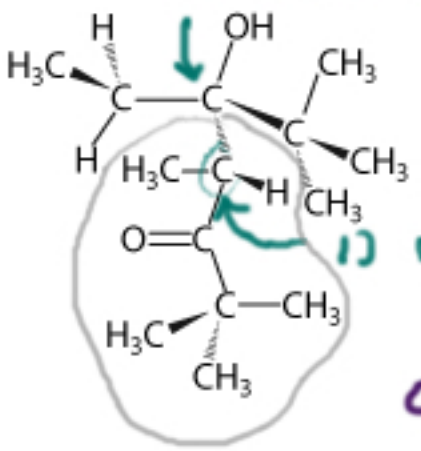


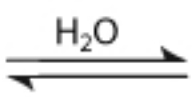




to work backwards

Find the carbon it attached

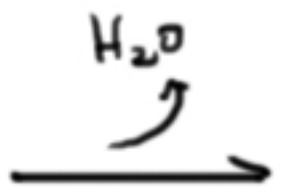




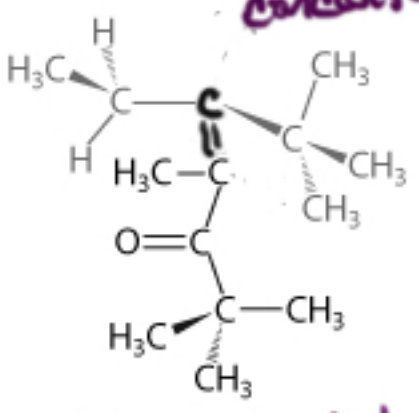
+ OH⁻

1) Find the original α carbon

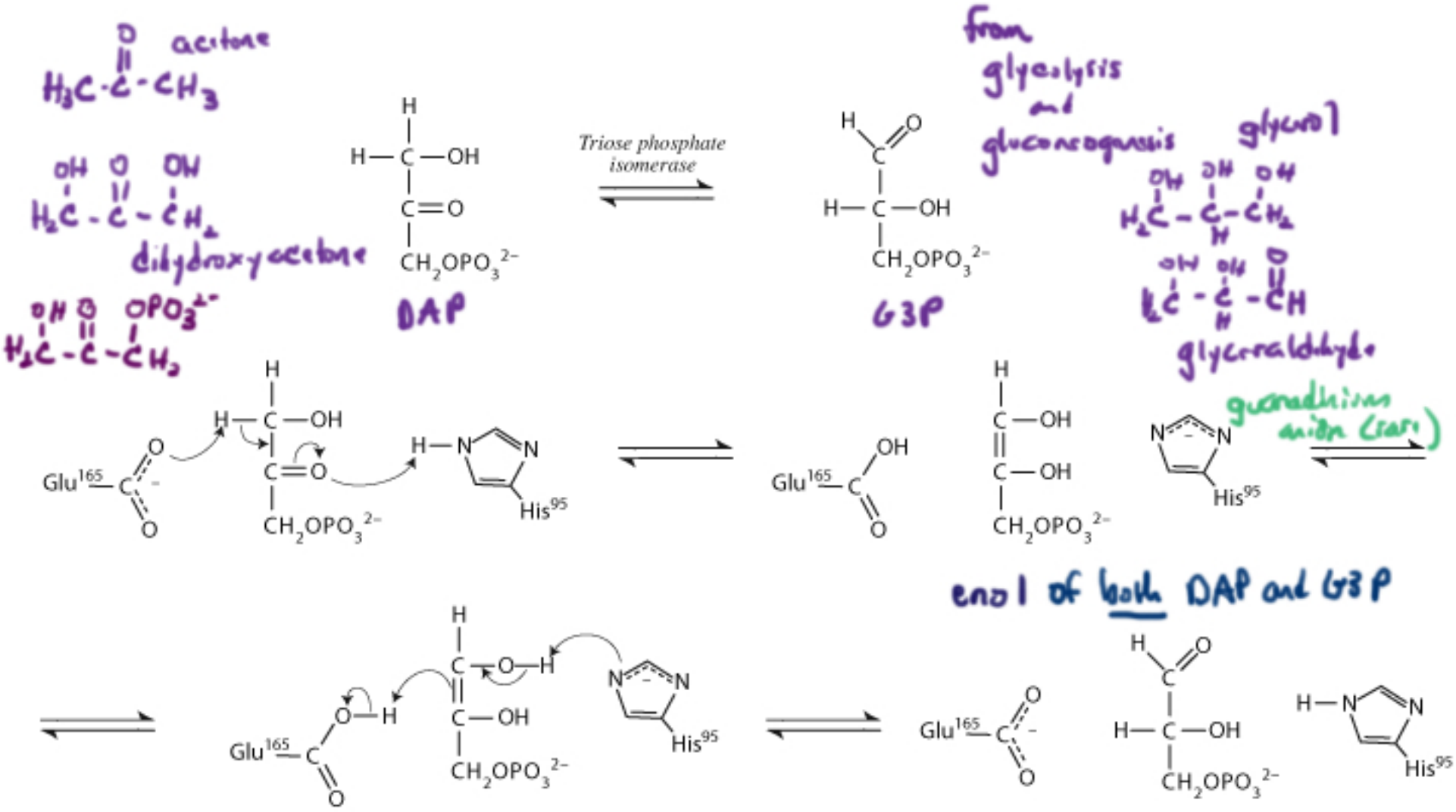
aldol addition product



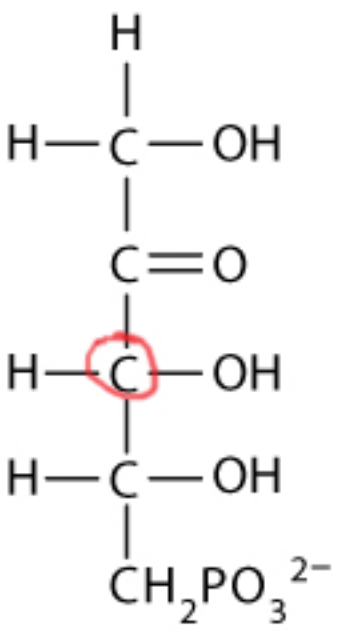
aldol condensation product



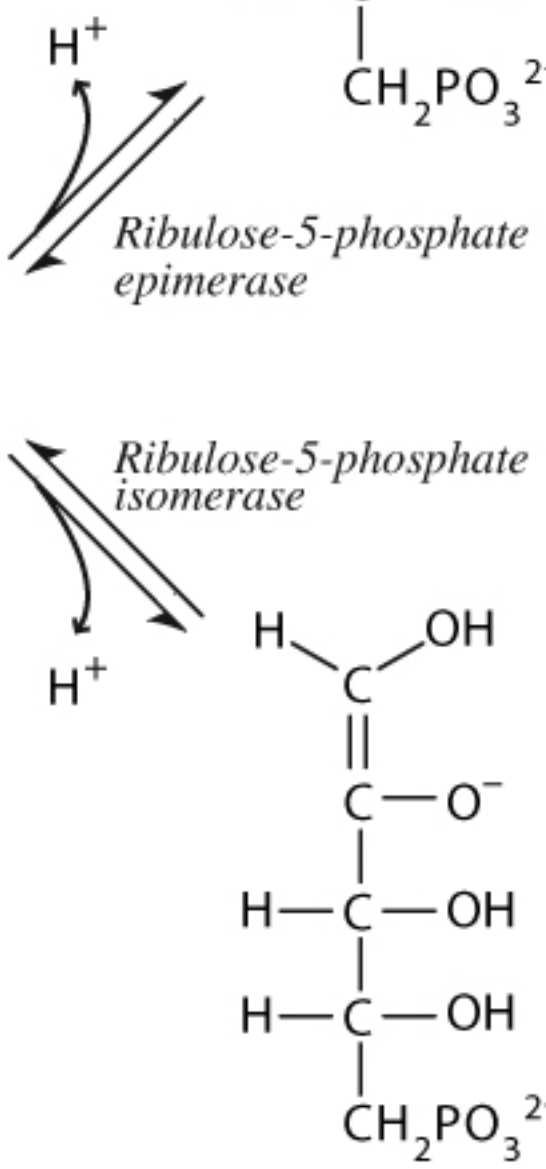
α,β unsaturated carbonyl compound


acetone
dihydroxyacetone
DAP
Triose phosphate isomerase
G3P
from glycolysis and gluconeogenesis
glycerol
glyceraldehyde
guanidinium anion (resn)
end of both DAP and G3P
Glu165
His95

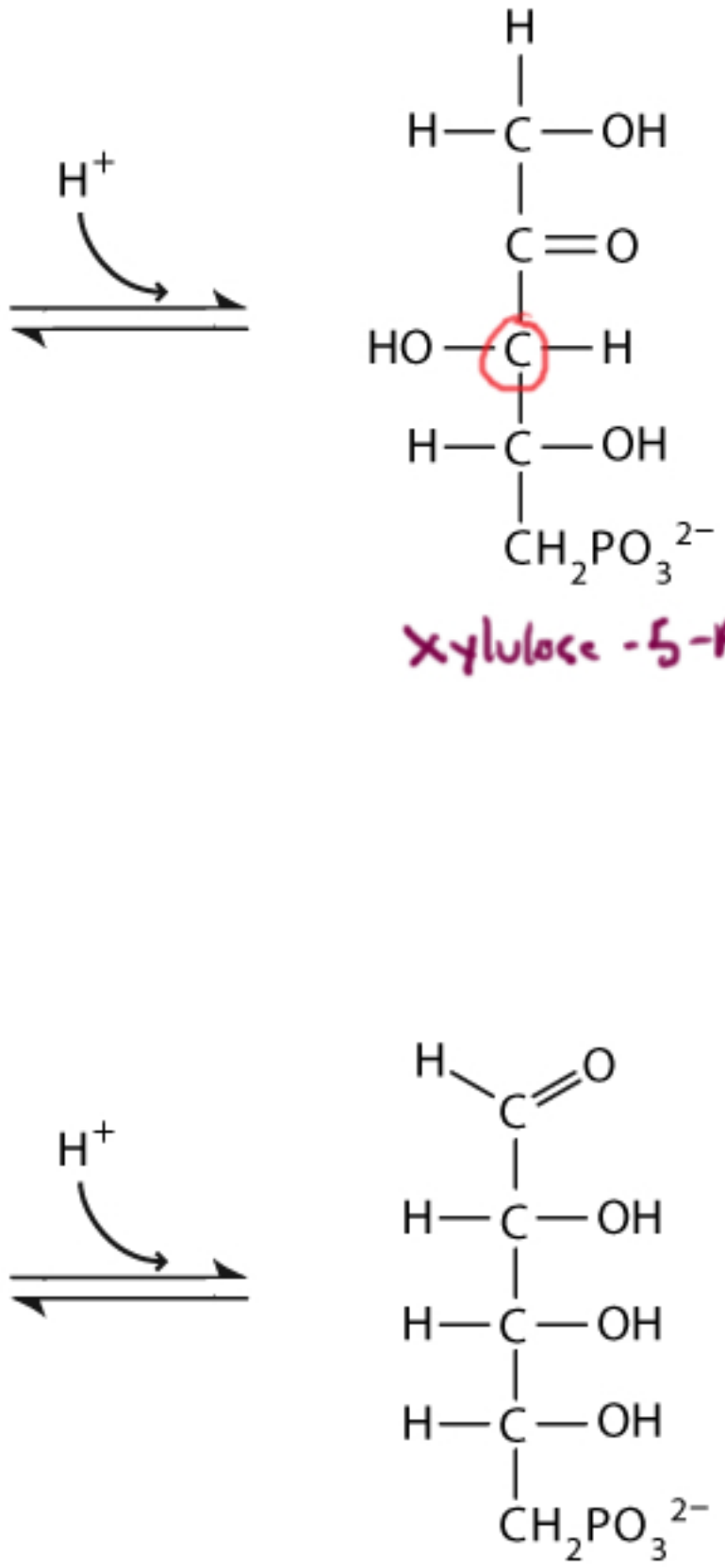
From pentose phosphate pathway (primary source of NADPH and ribose)



ribulose 5-P



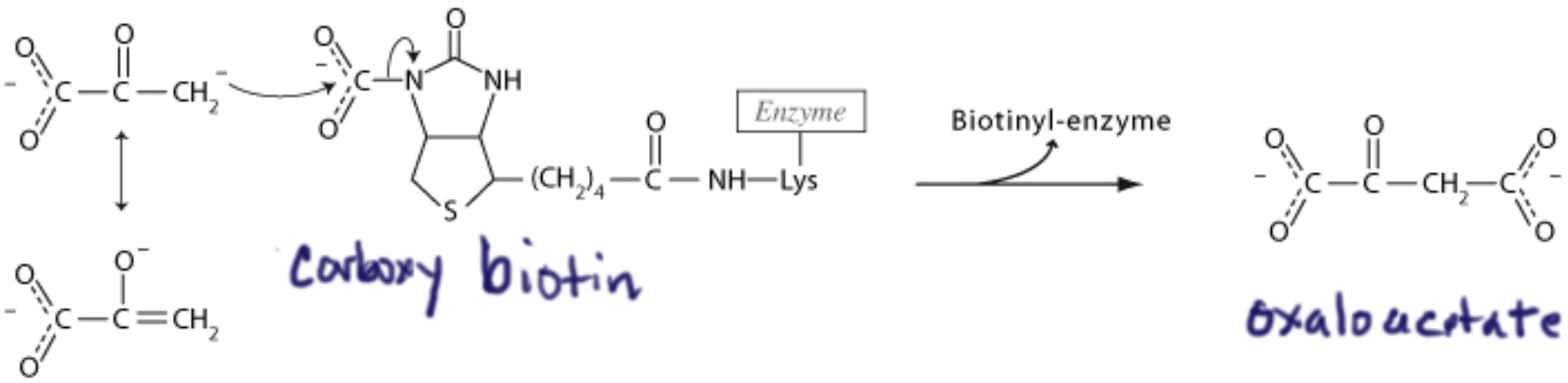
enol of both



Xylulose -5-P

Ribose 5-P

pyruvate carboxylase



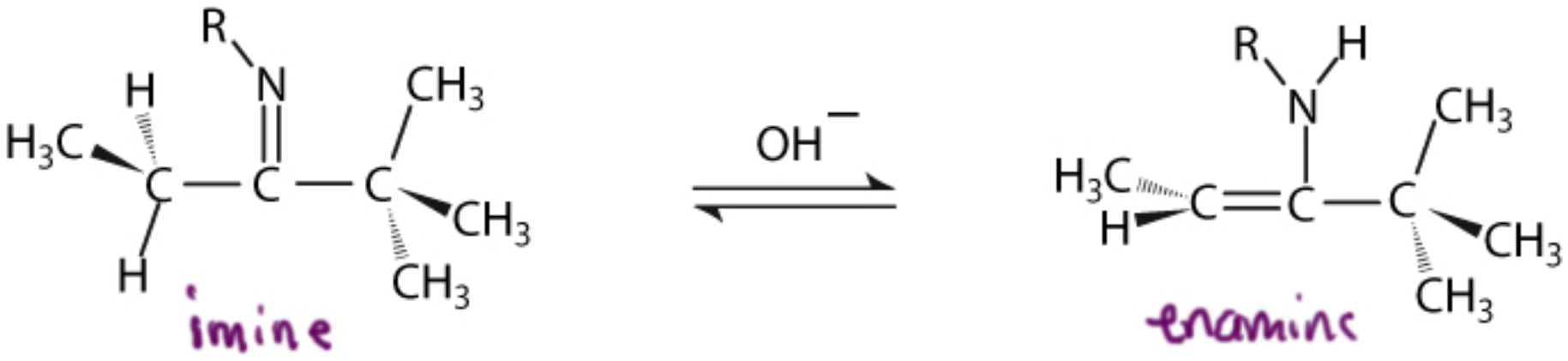
carboxy biotin

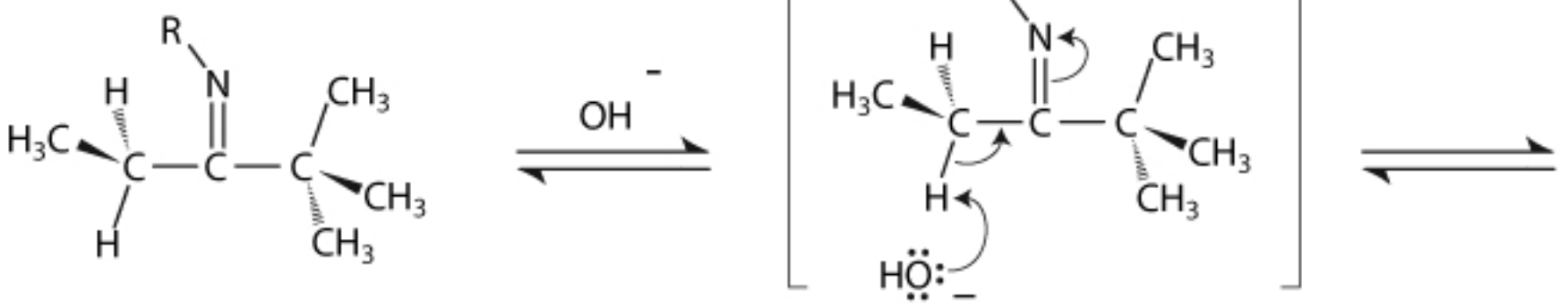
enolate of pyruvate

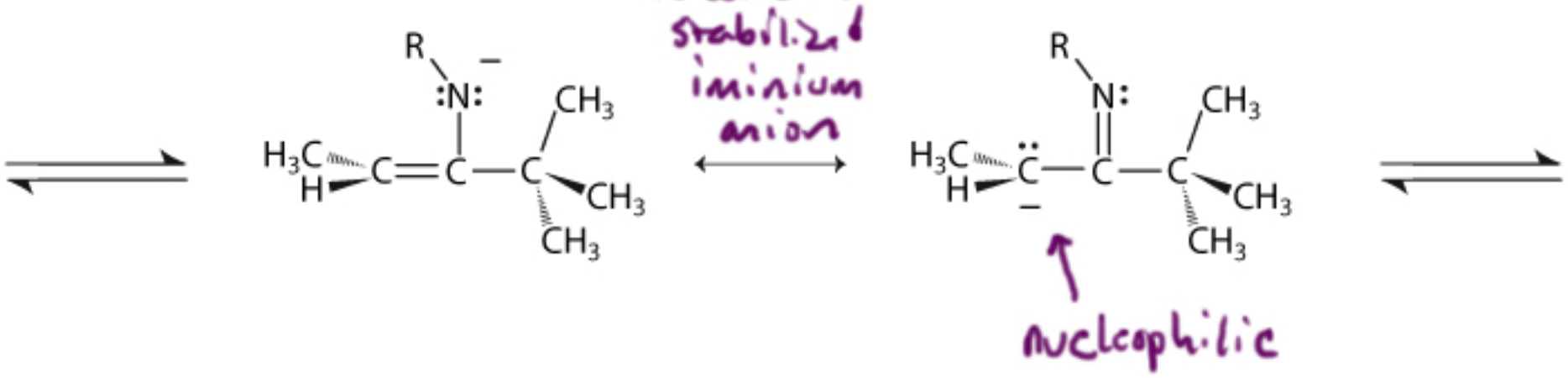
oxaloacetate

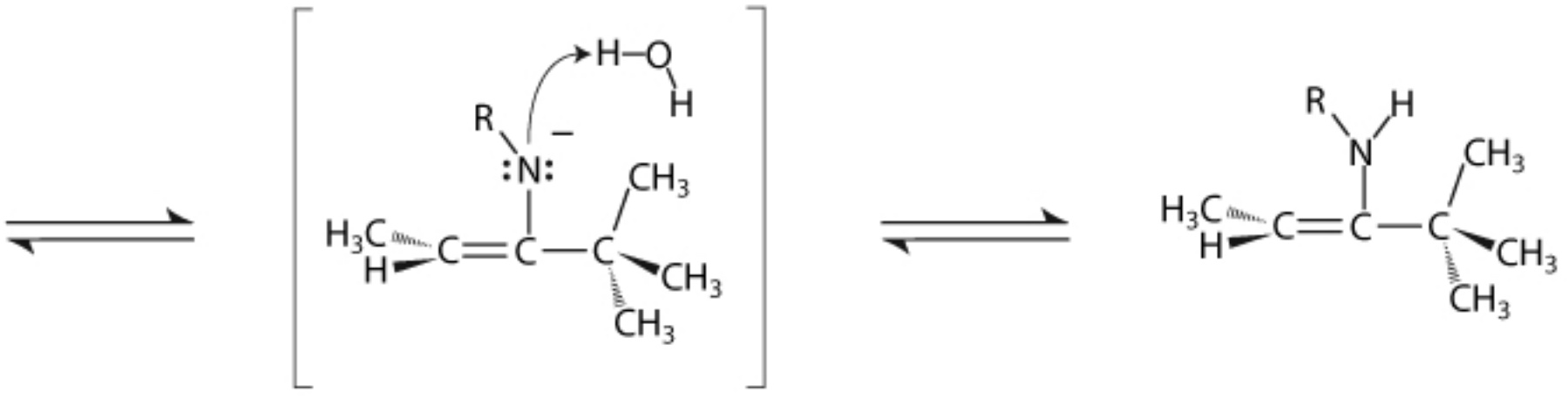
(biotin is a carboxyl donor)

imine enamine tautomerism

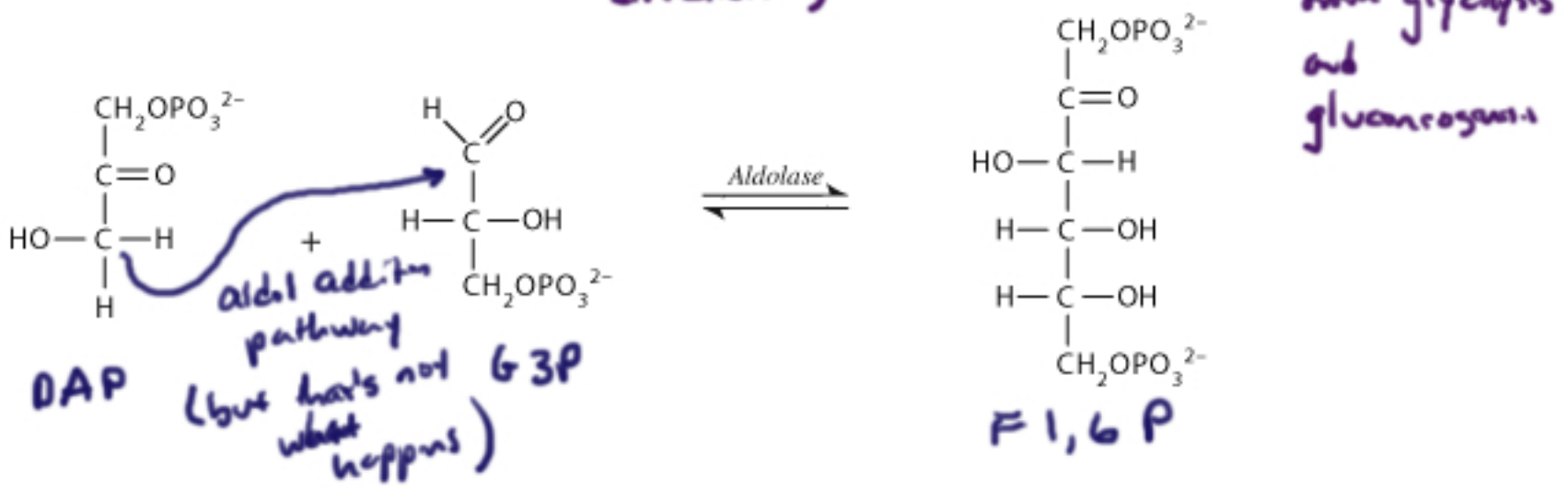


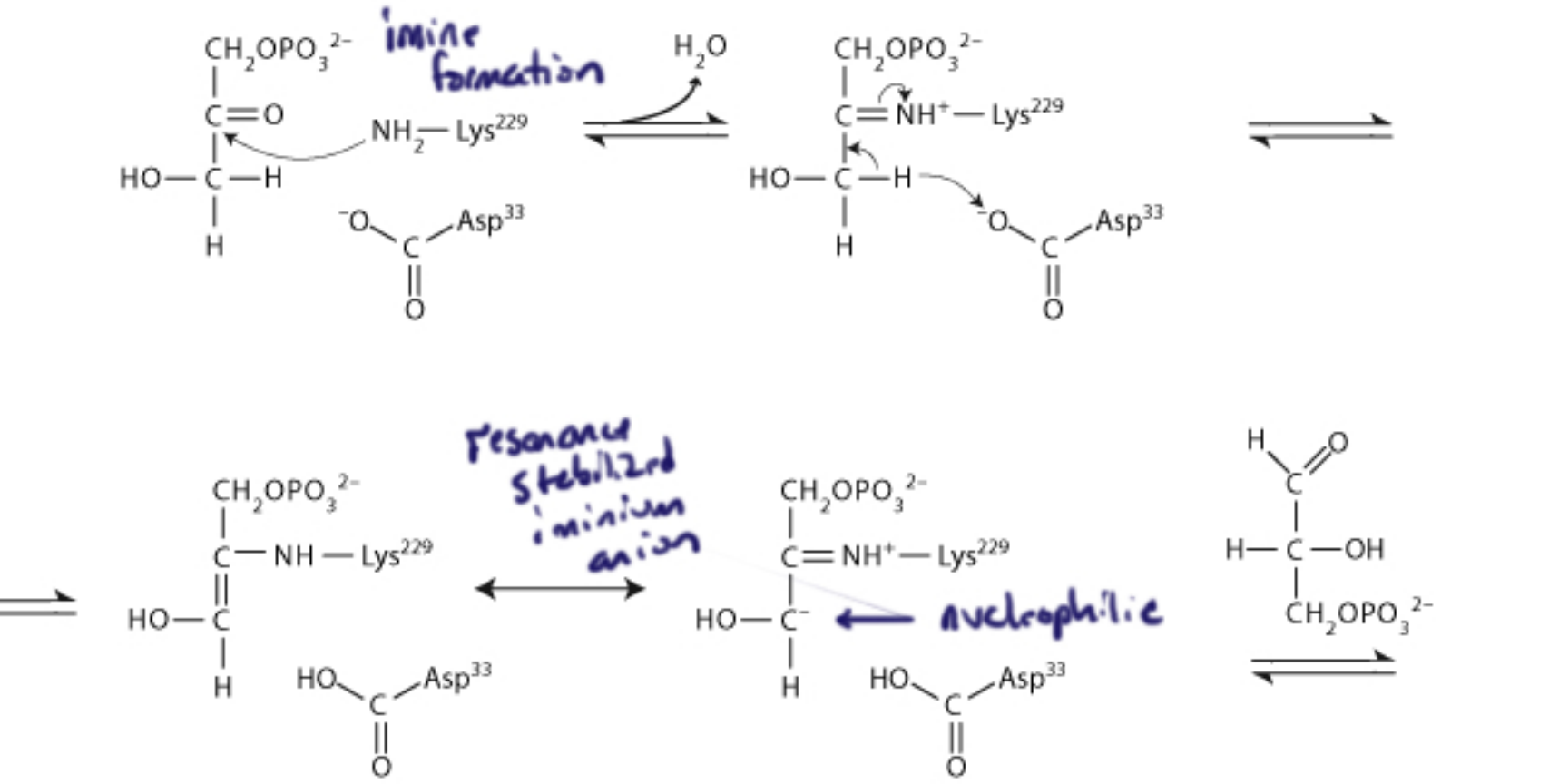


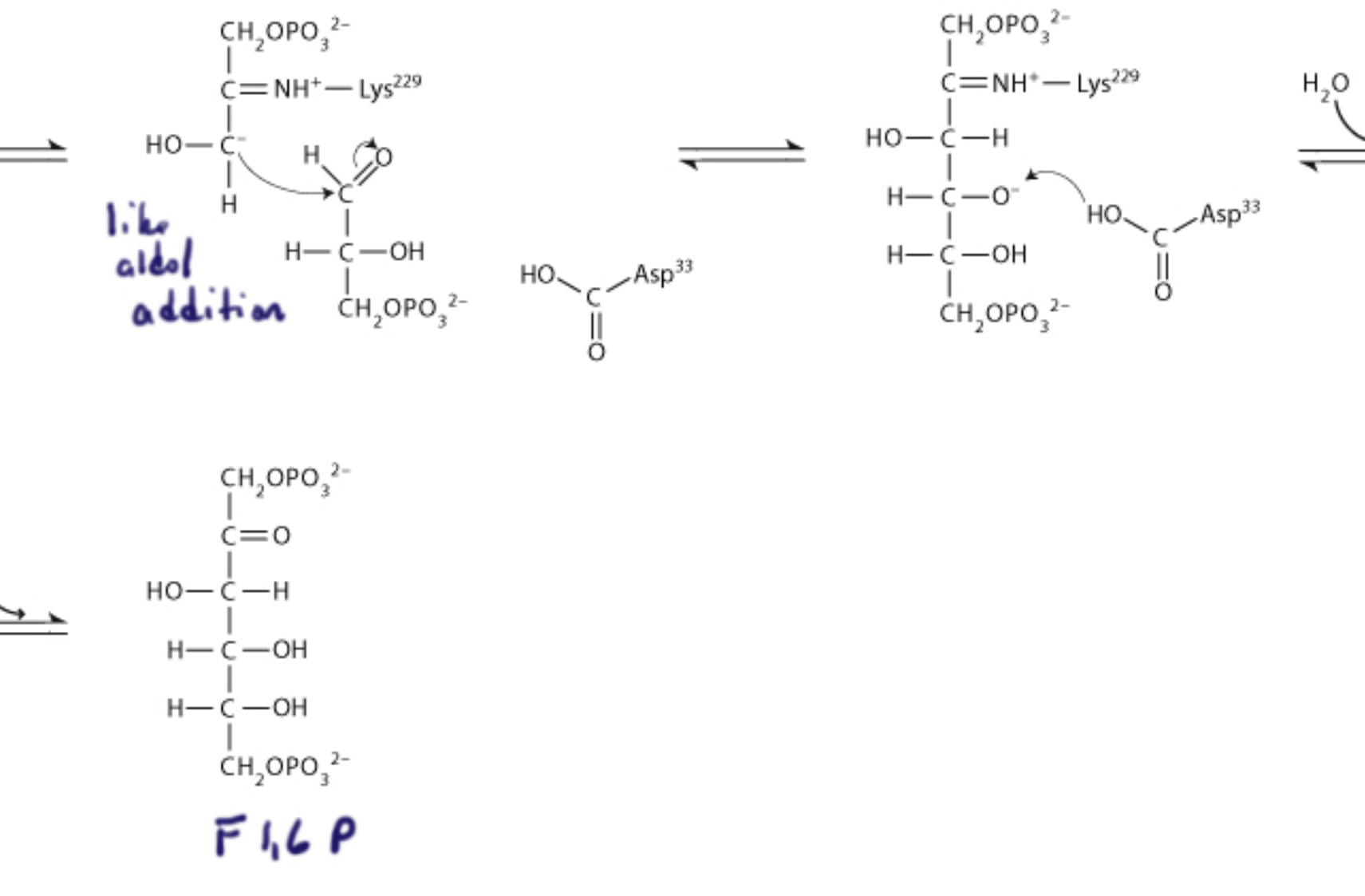




Aldolase (gluconeogenesis direction)



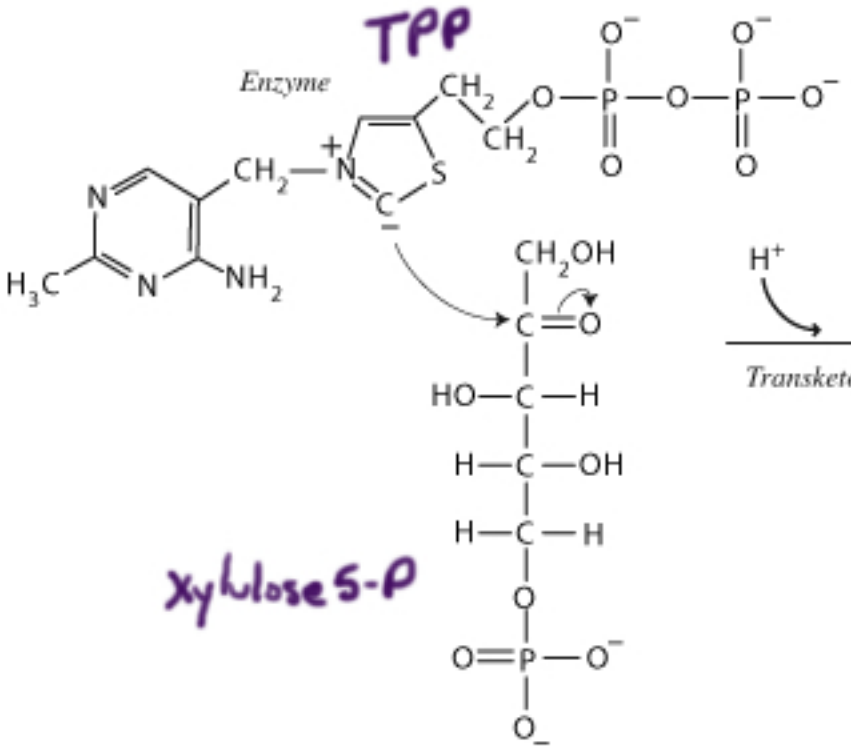




Transketolase (moves 2C)

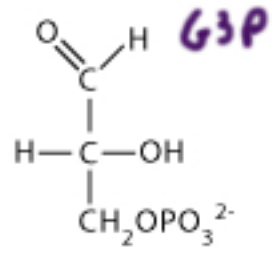
from PPP

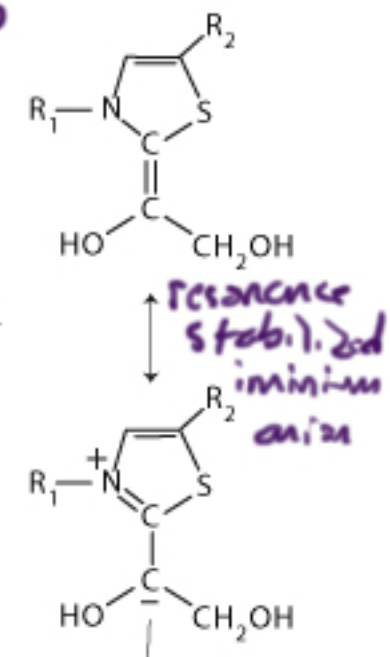
TPP



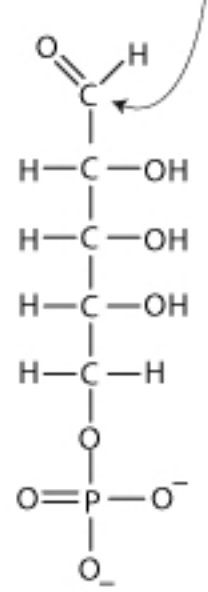
xylulose 5-P

G3P

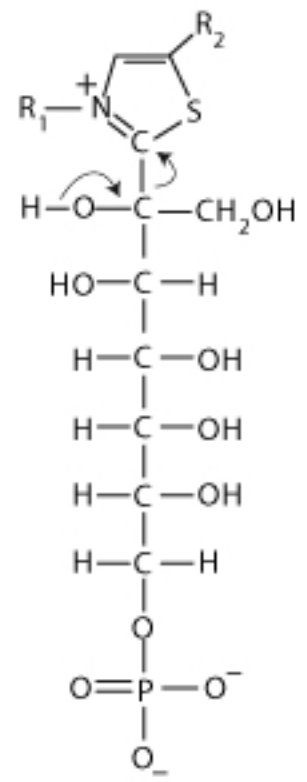




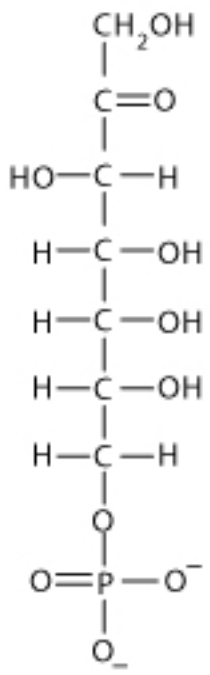
resonance stabilized iminium anion



like aldol addition



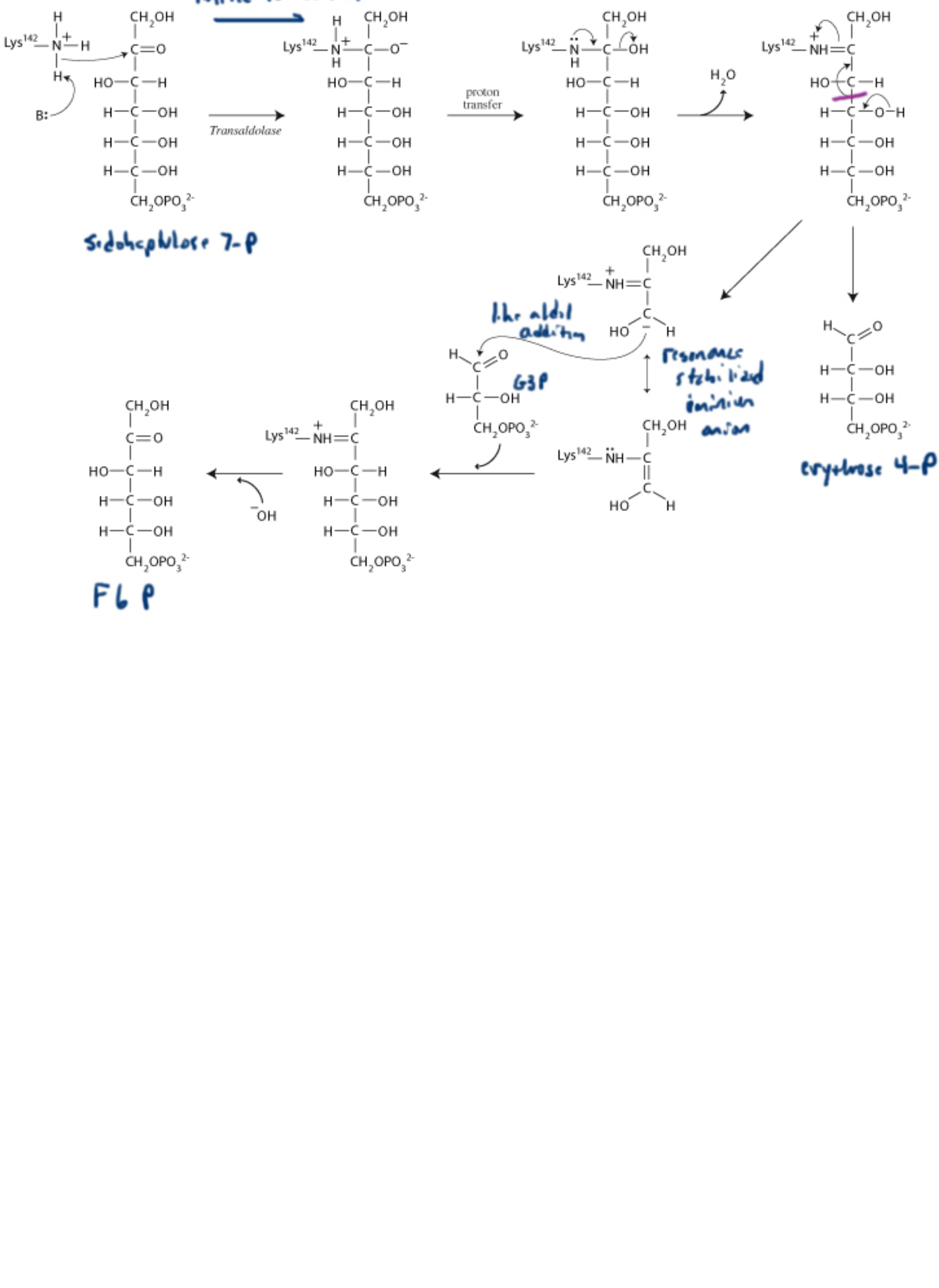
TPP



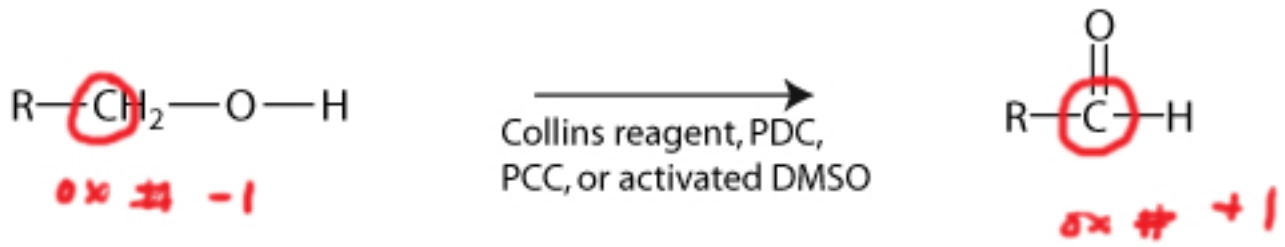
sed. heptulose 7-P

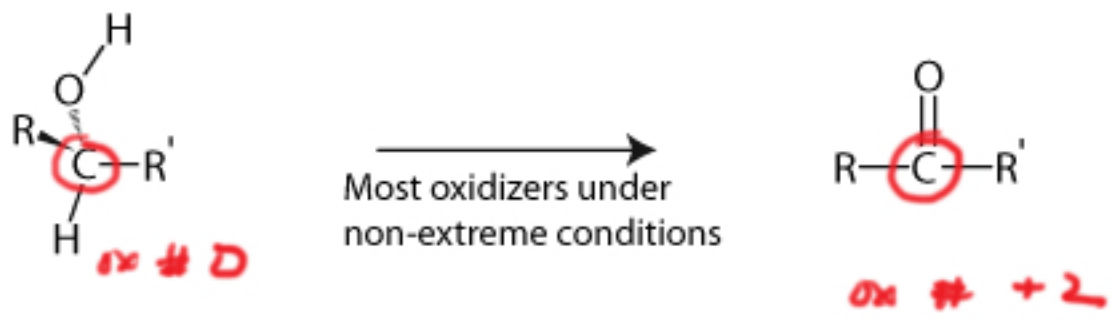
ribose 5-P

Transaldolase (moves 3C)

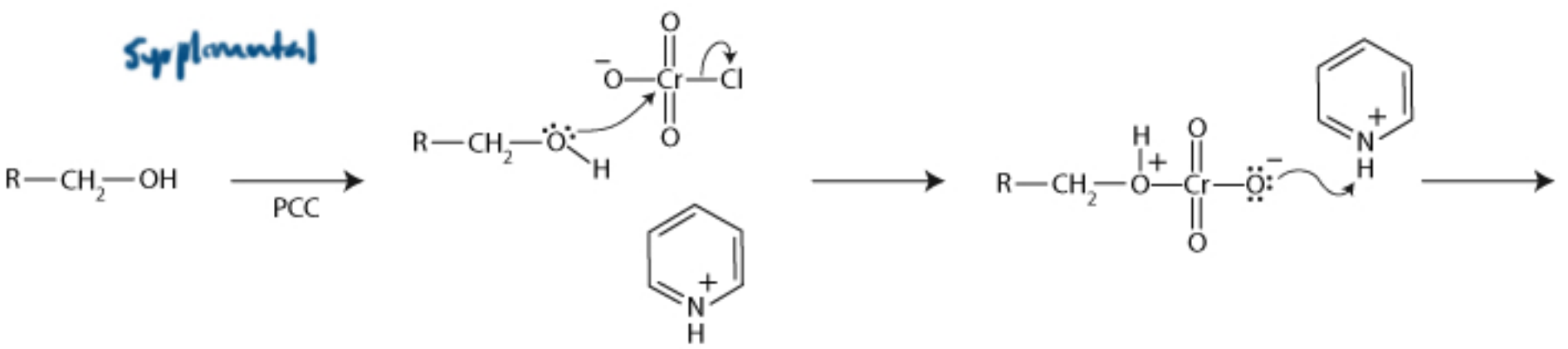


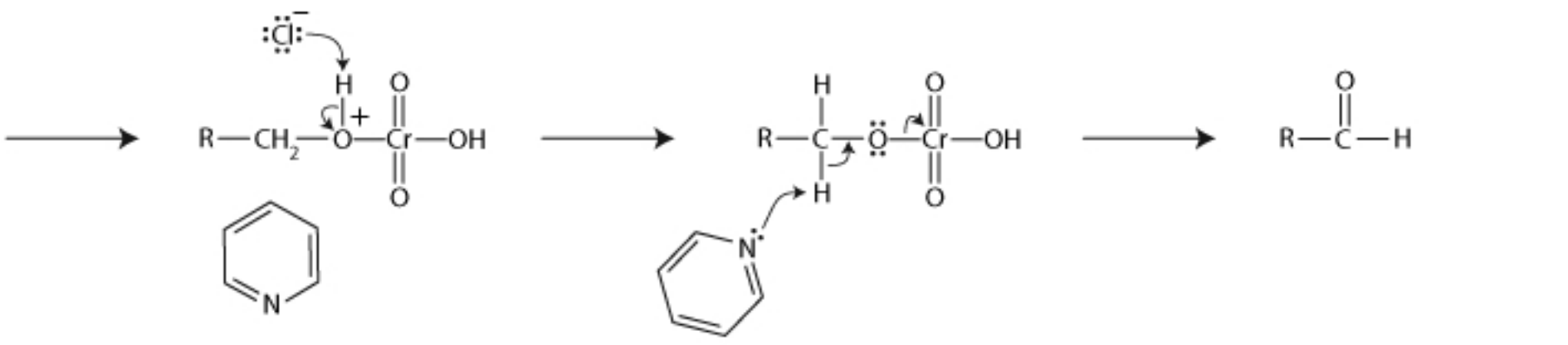
Oxidation of Alcohols





Supplemental

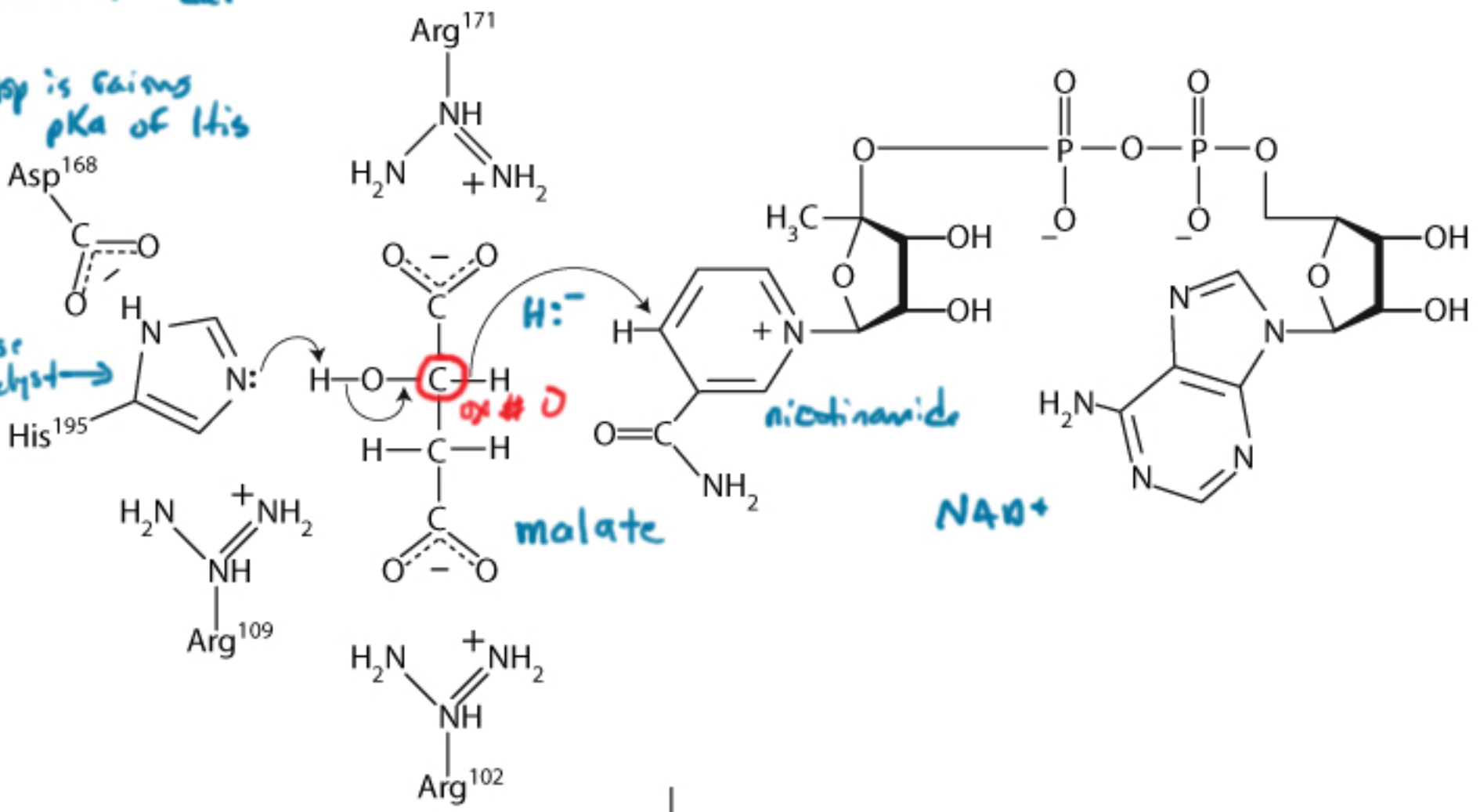




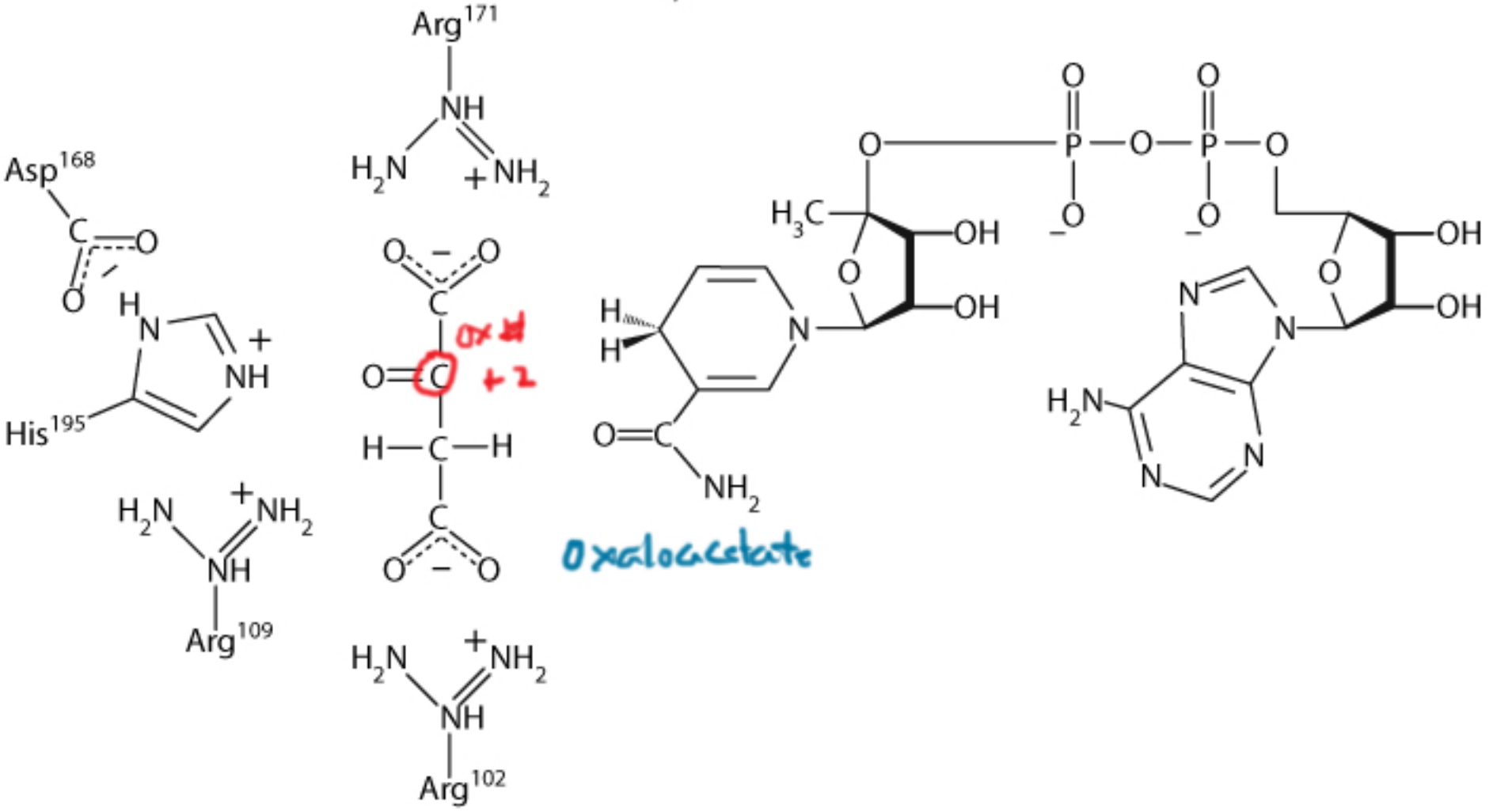
D168A
would change k_{cat}

malate dehydrogenase

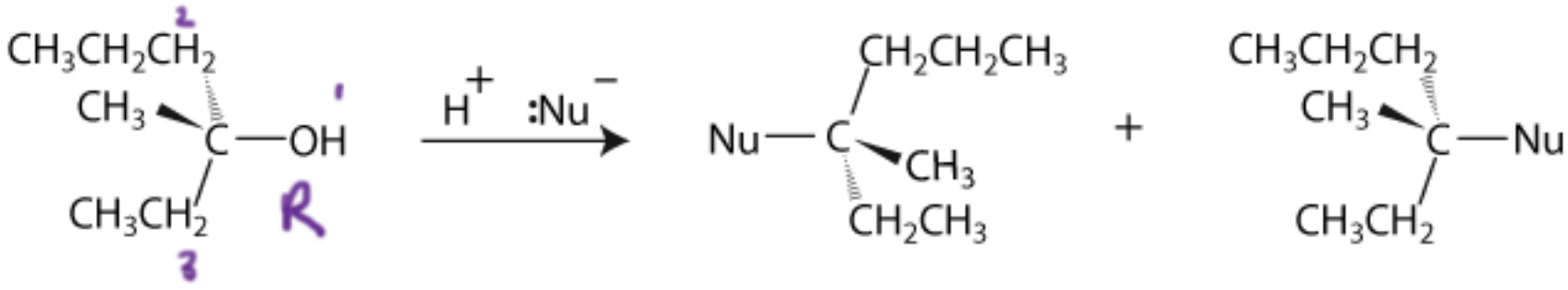
Asp is raising pKa of this



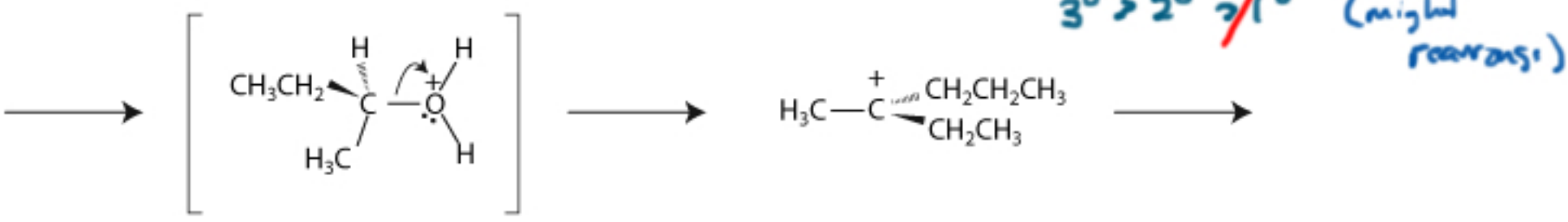
R102A
if we substituted with an alanine, would change K_M



SN1 Substitution



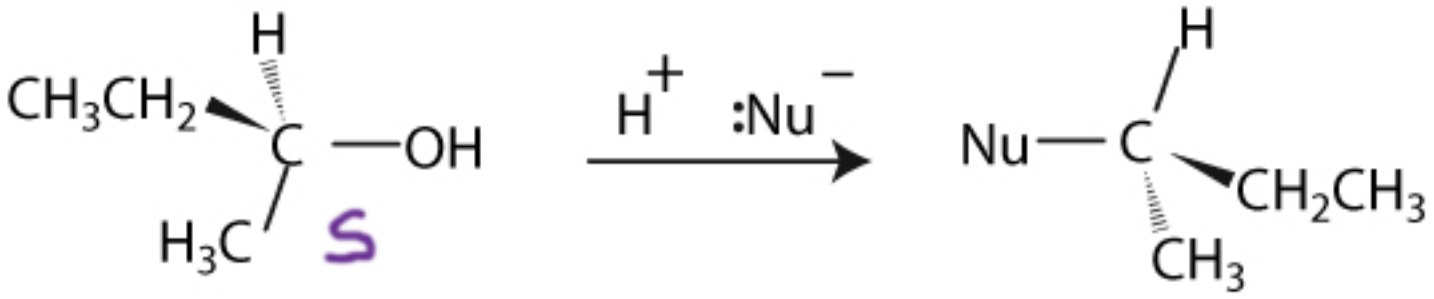
poor leaving group



3° > 2° ~~>~~ 1° (might rearrange)

racemic mixture
(not optically active)

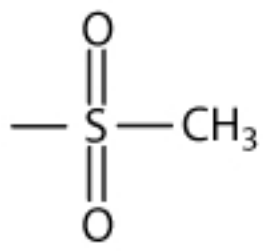
SN2

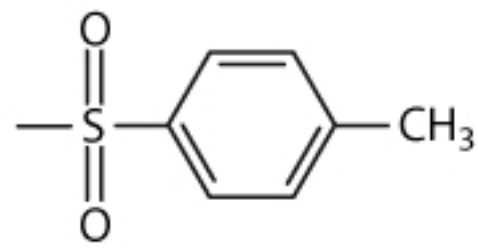


- prefers unhindered nucleophile and substrate
- polar aprotic solvent

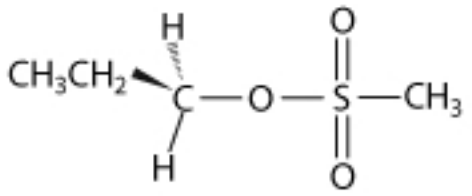
stereospecific for inversion of configuration

Mesylate and tosylate leaving group

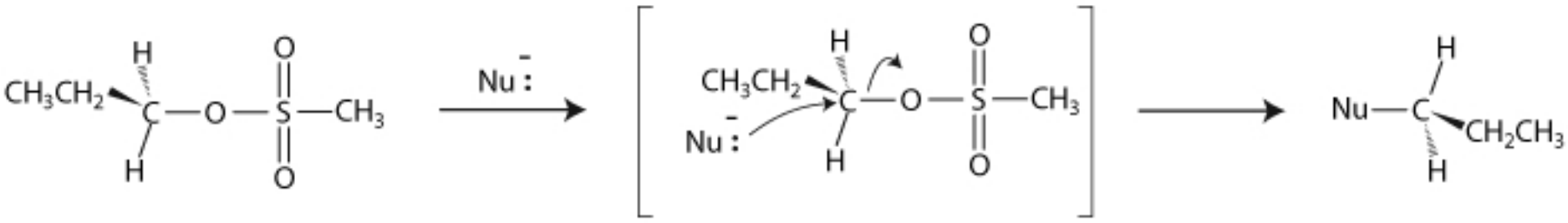




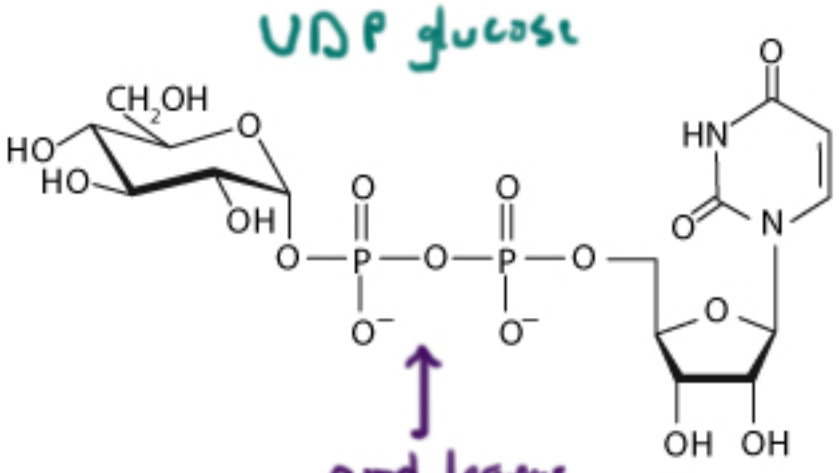
poor leaving group



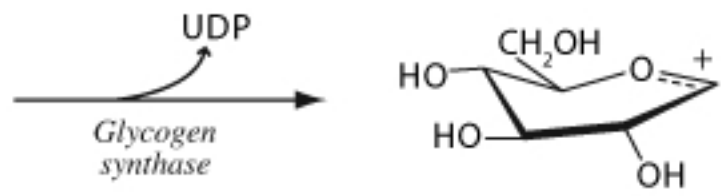
good leaving group



UDP glucose

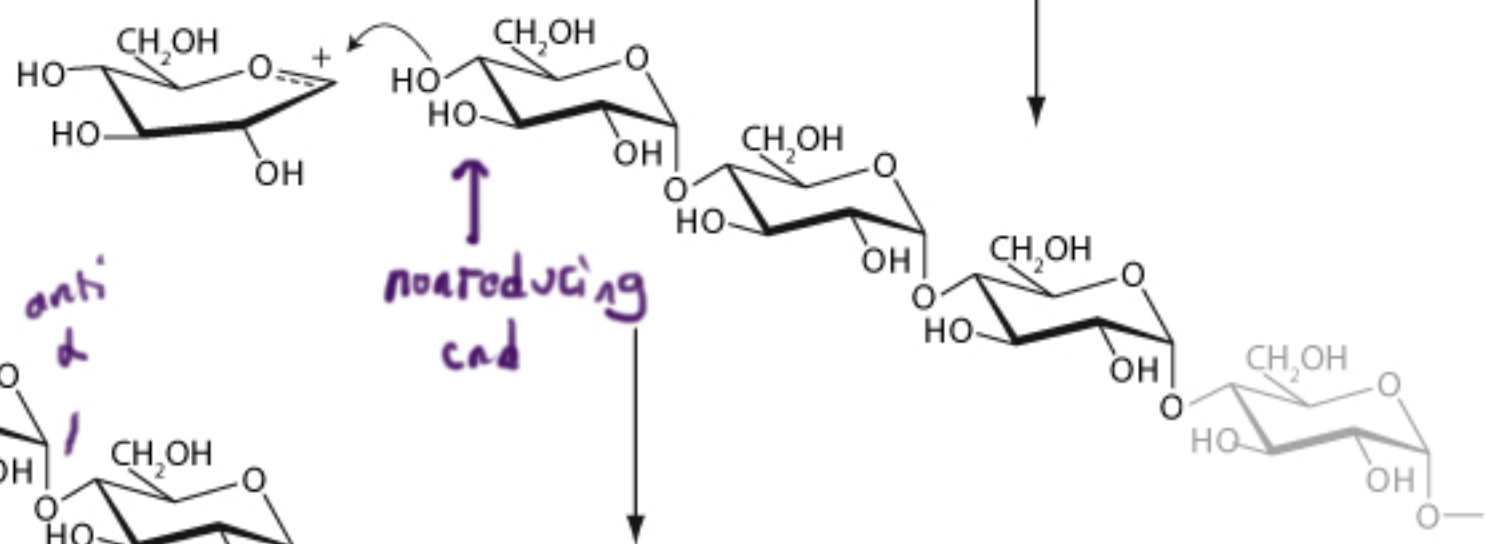


good leaving group

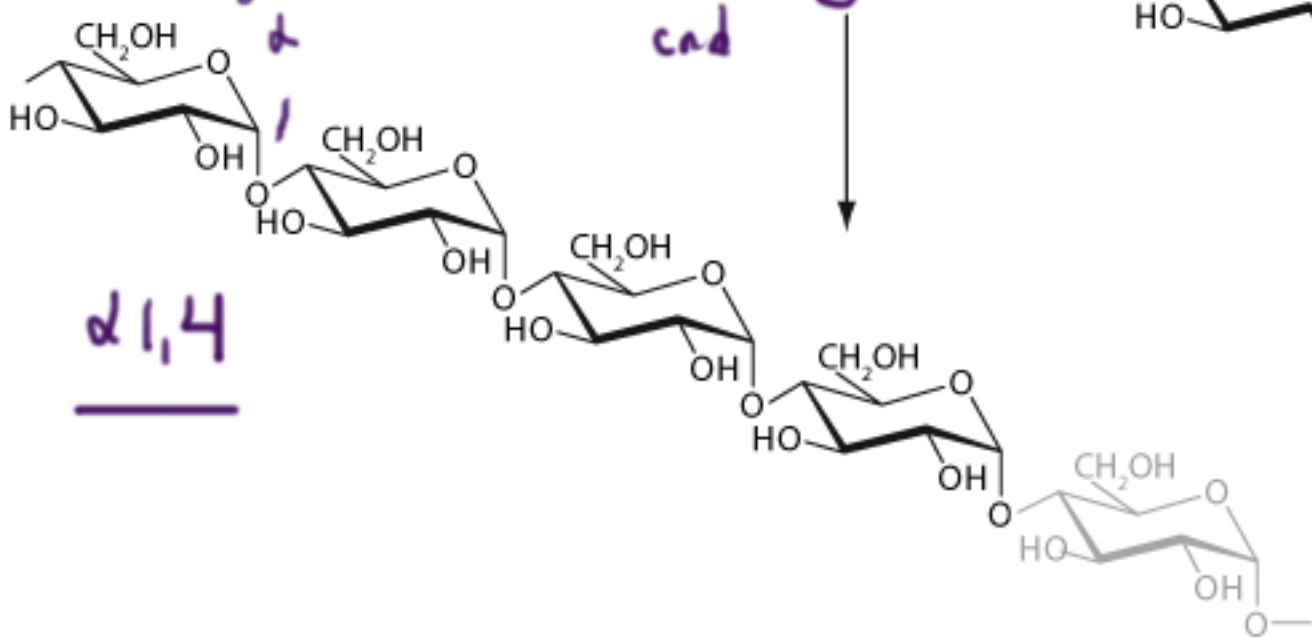


Oxonium cation

like step 2 of acetal formation

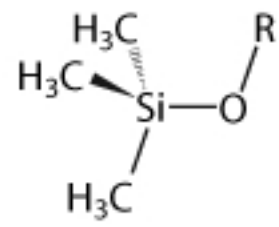


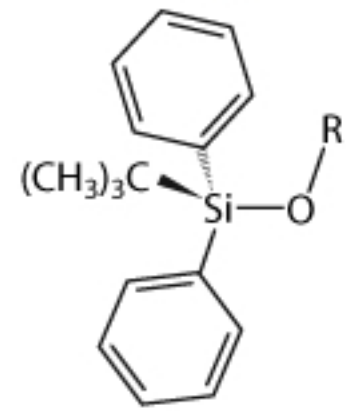
nonreducing end

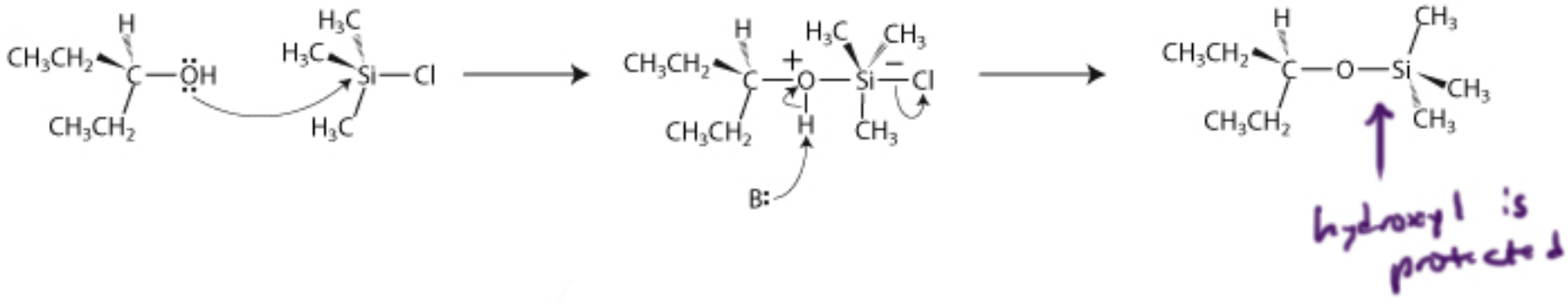


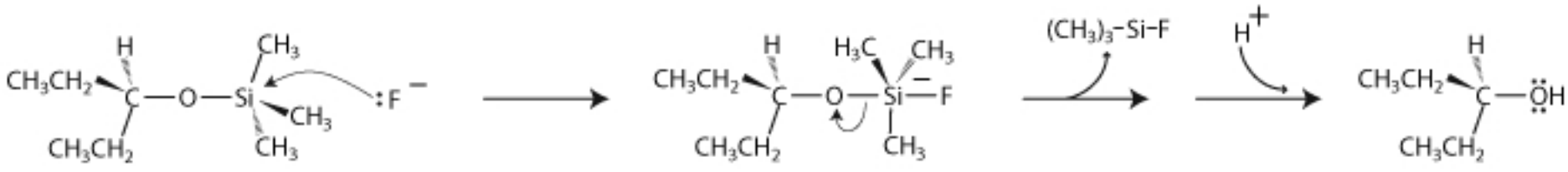
α 1,4 — anti

Silyl Protecting Group





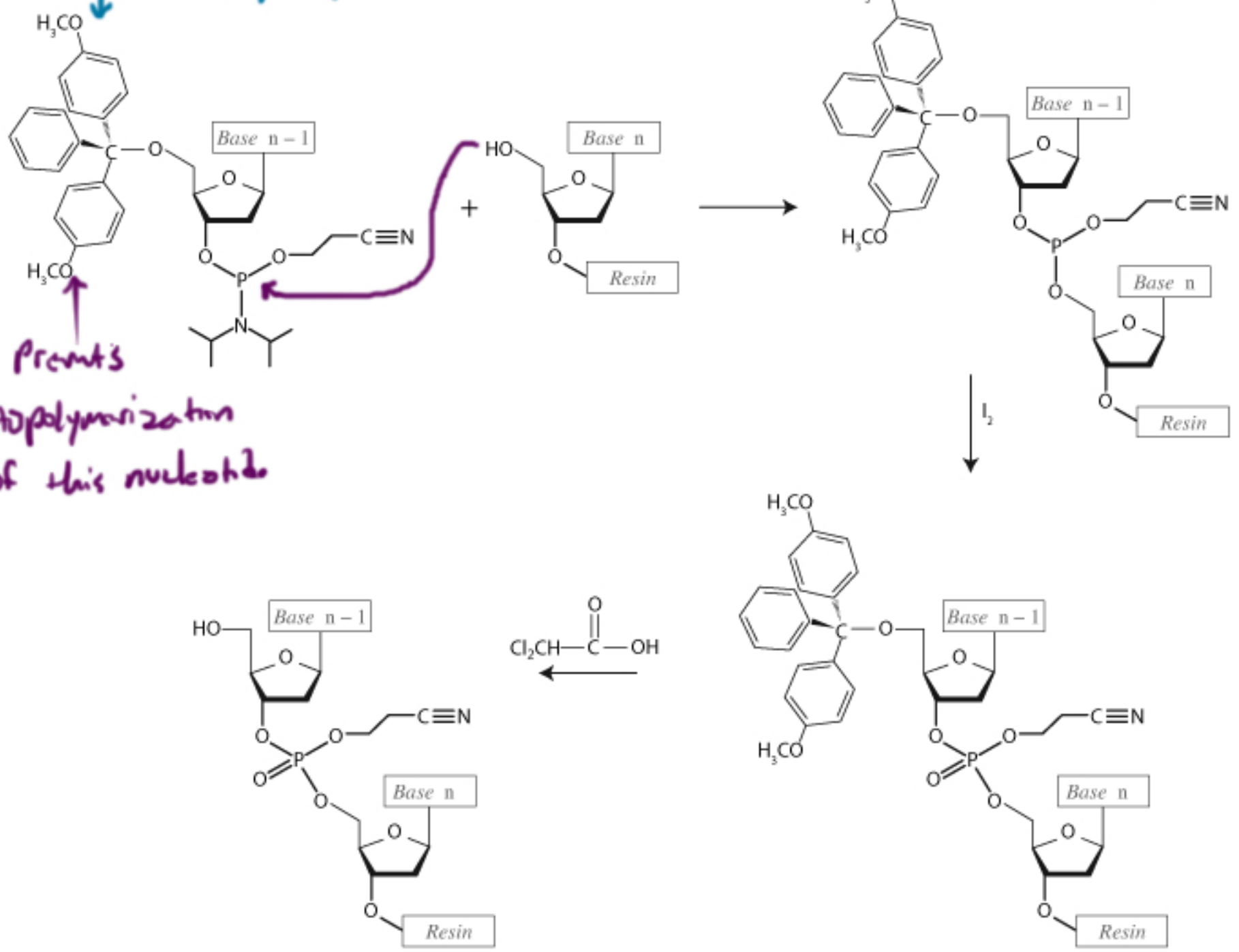




DMT
dimethoxytrityl

DMT protecting group

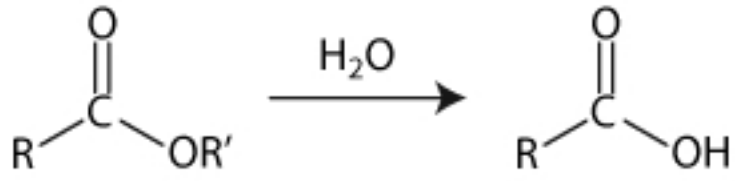
Solid Phase DNA Synthesis



Prevents autopolymerization of this nucleotide

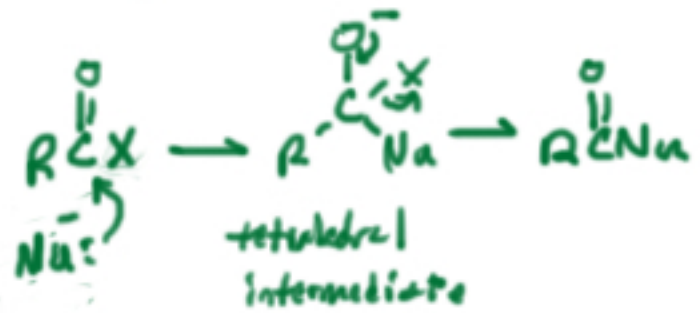
Carboxylic Acid Derivatives

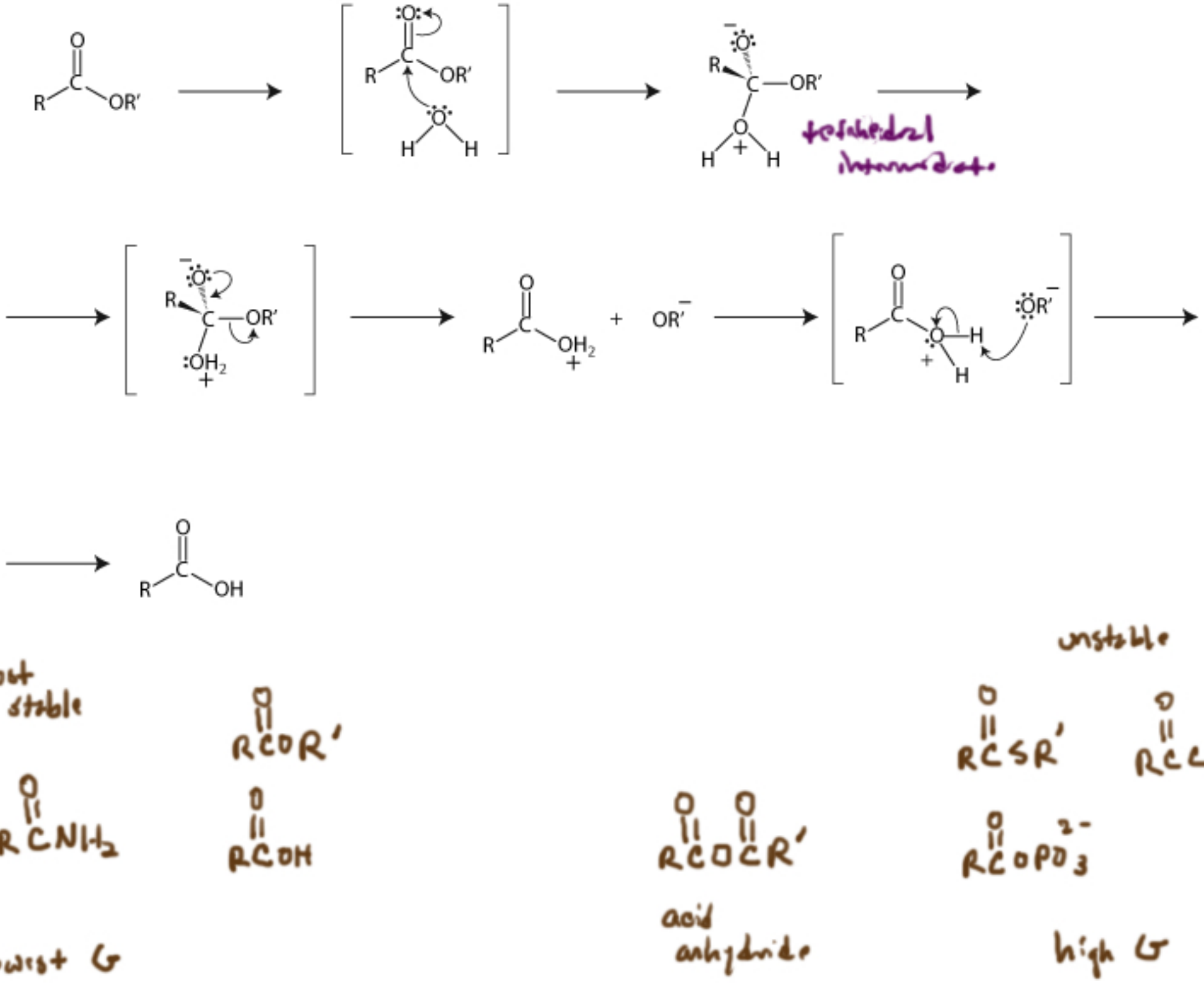
Hydrolysis of an Ester



Ester → Carboxylic Acid

Nucleophilic Acyl Substitution





Most stable

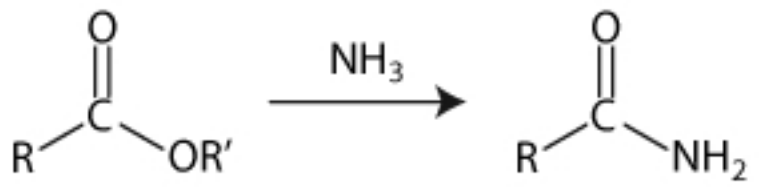
acid anhydride

unstable

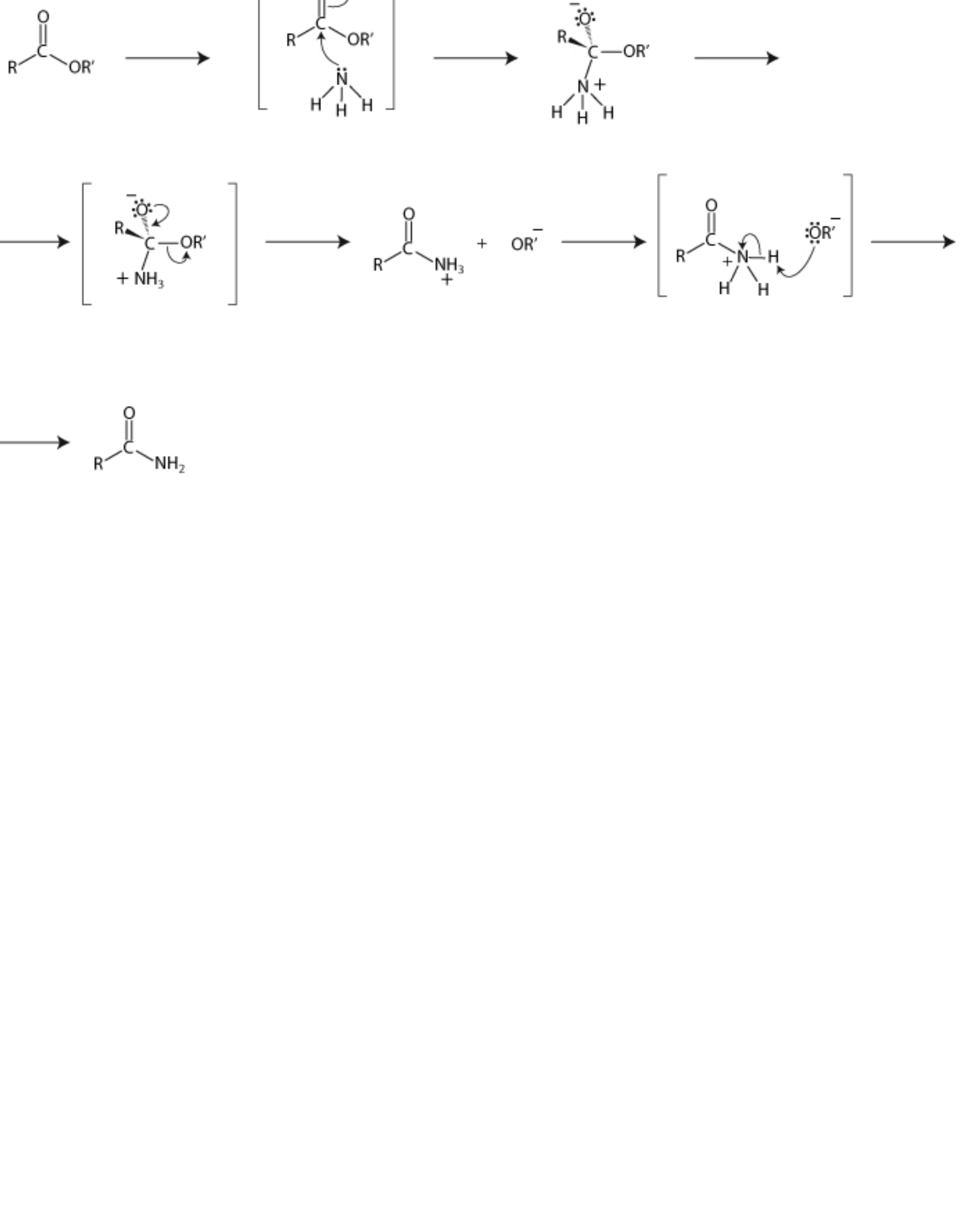
lowest G

high G

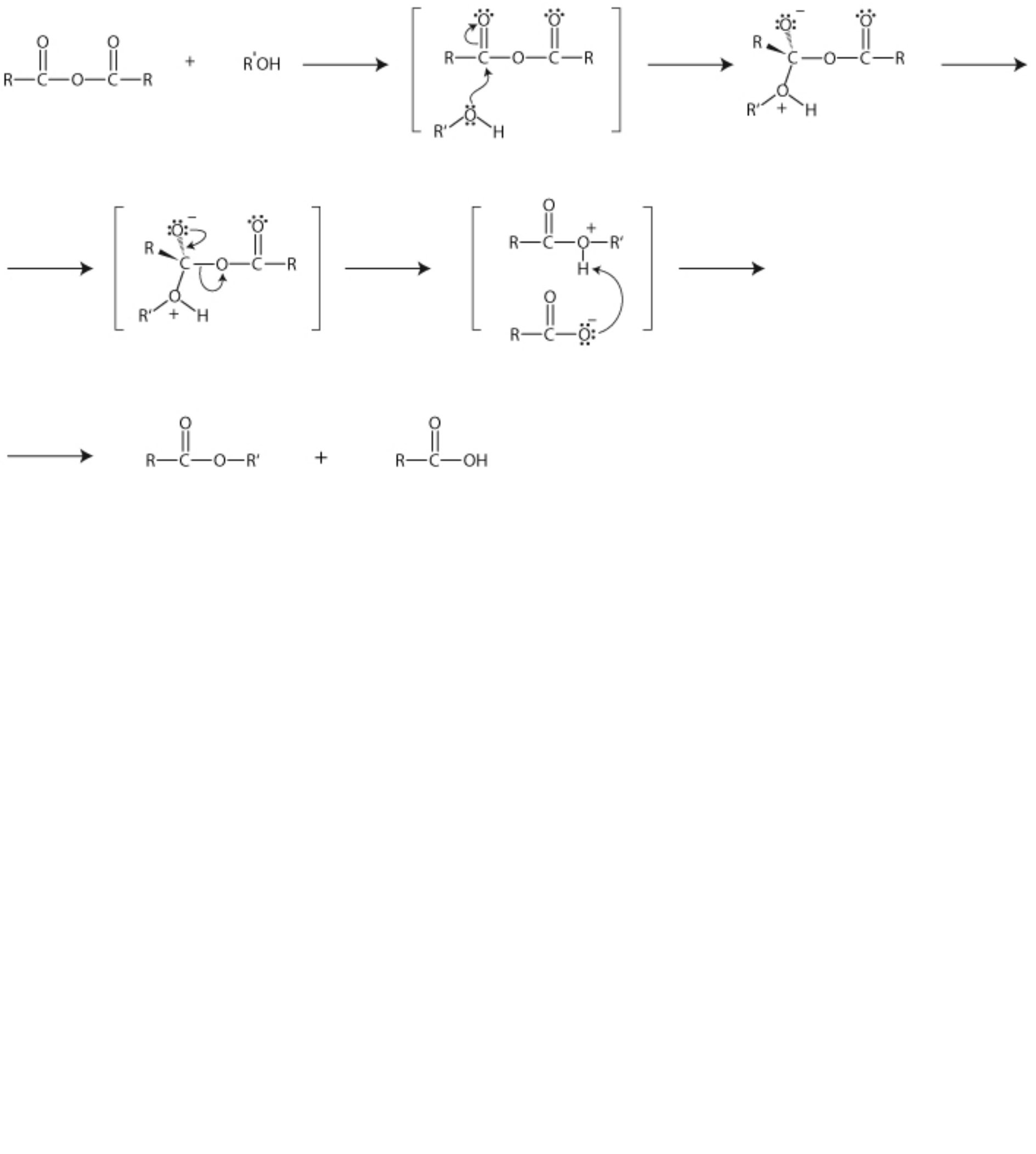
Aminolysis of Ester



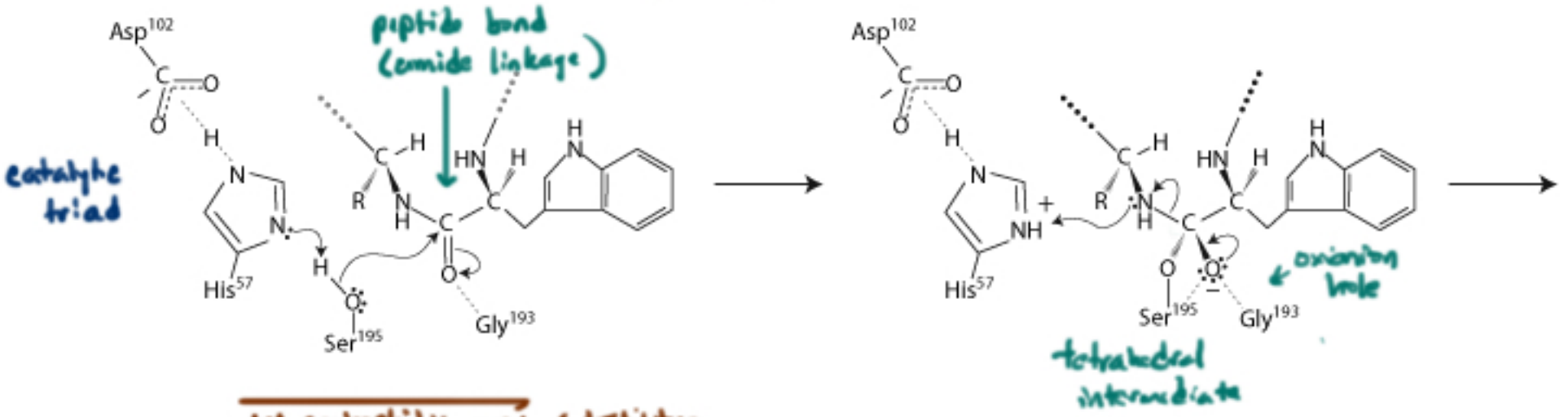
Ester → Amide



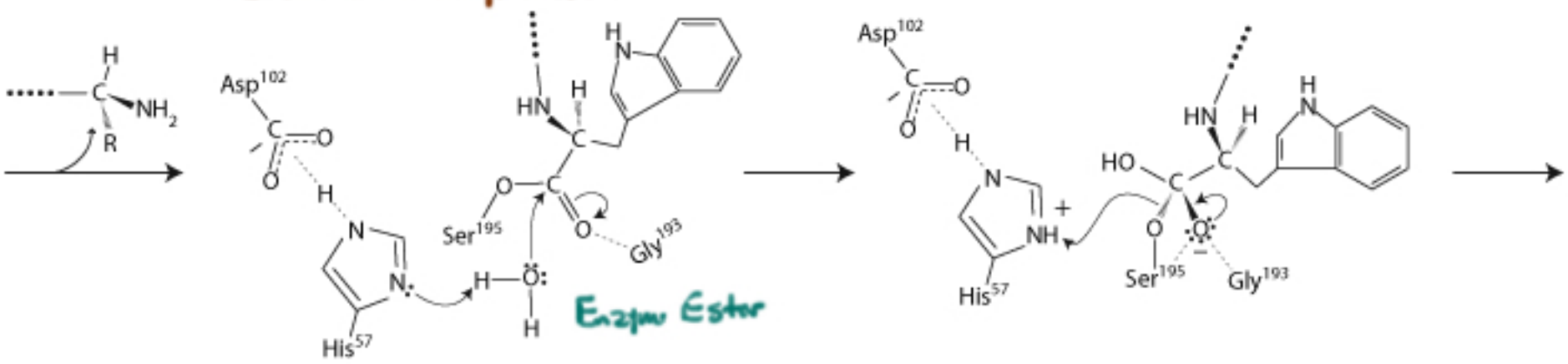
Esterification of an Anhydride



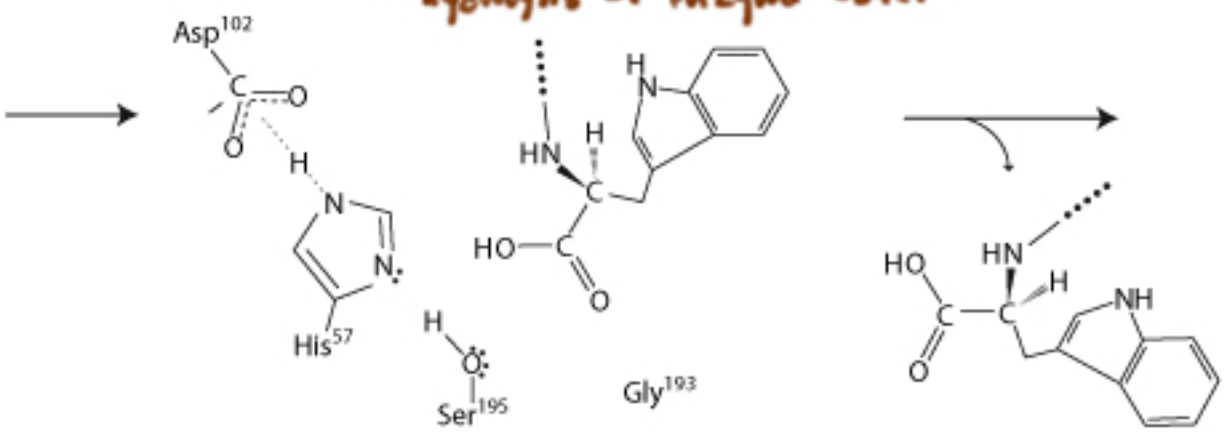
Chymotrypsin - A serine protease



1st nucleophilic acyl substitution
- formation of enzyme ester

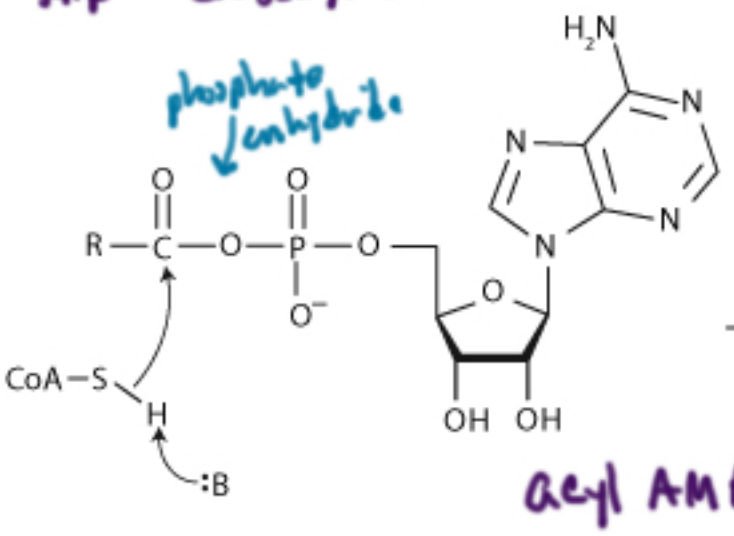


2nd acyl substitution
- hydrolysis of enzyme ester



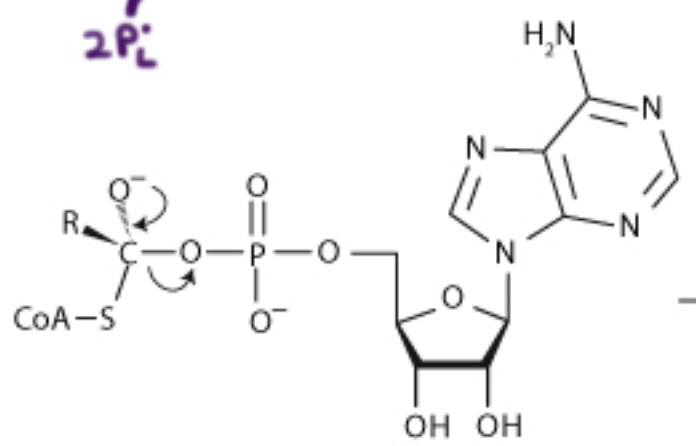
previous step : fatty acyl carboxylate + ATP → acyl AMP + PP_i → 2 P_i

Fatty Acid Activation



Acyl AMP

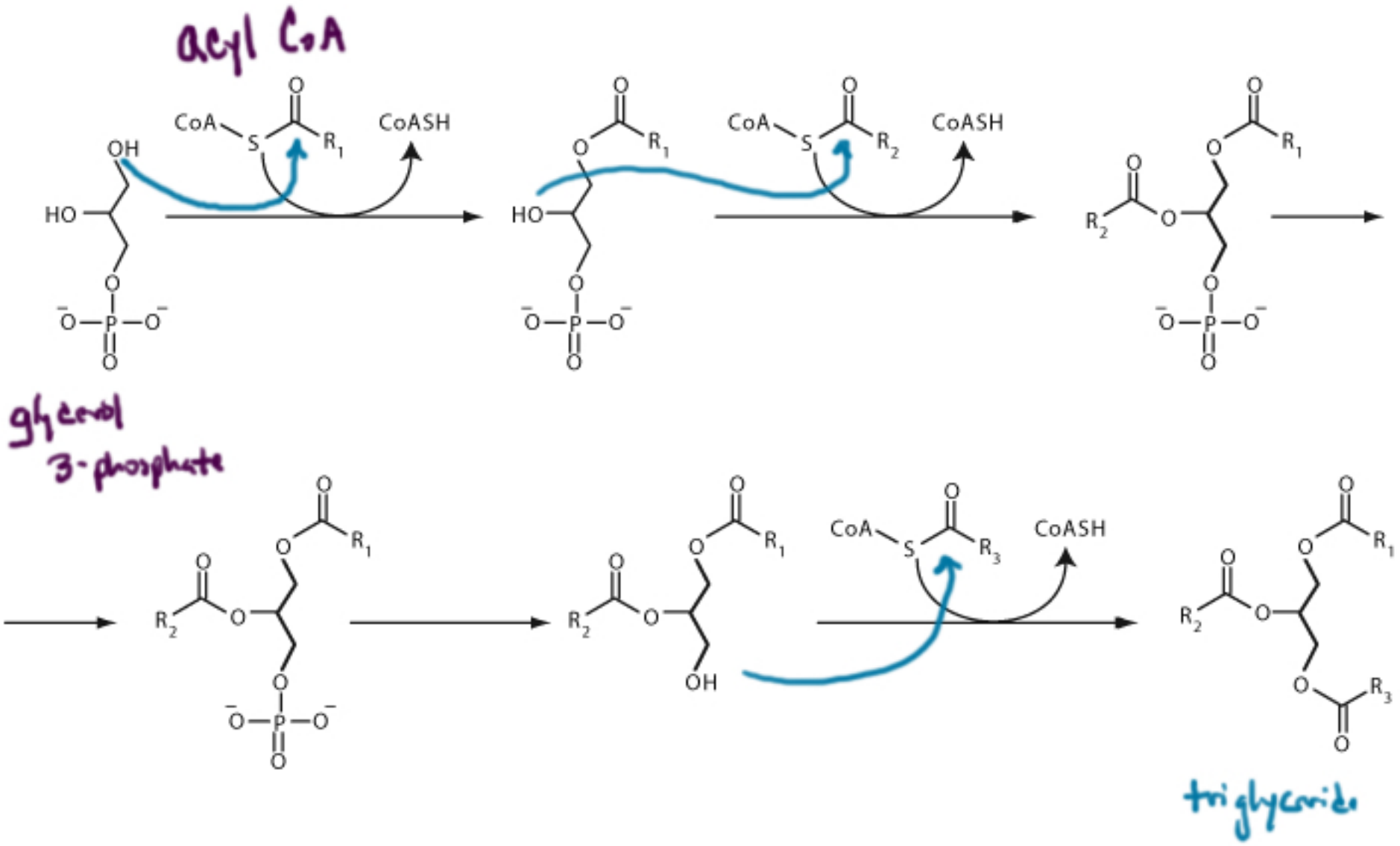
Acyl Coa synthetase →



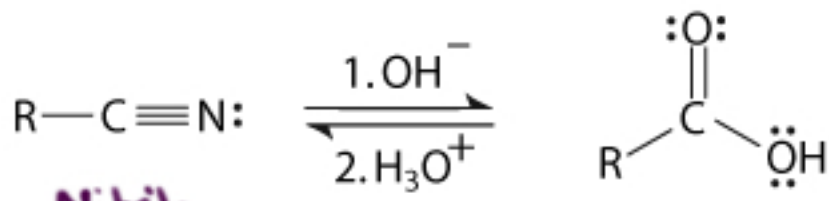
Acyl Coa synthetase →

Acyl Coa synthetase →

Fatty Acyl CoA


acyl CoA
CoA
S
R1
CoASH
OH
HO
O
P
O
glycerol
3-phosphate
R2
R3
triglyceride

Nitrile Hydrolysis

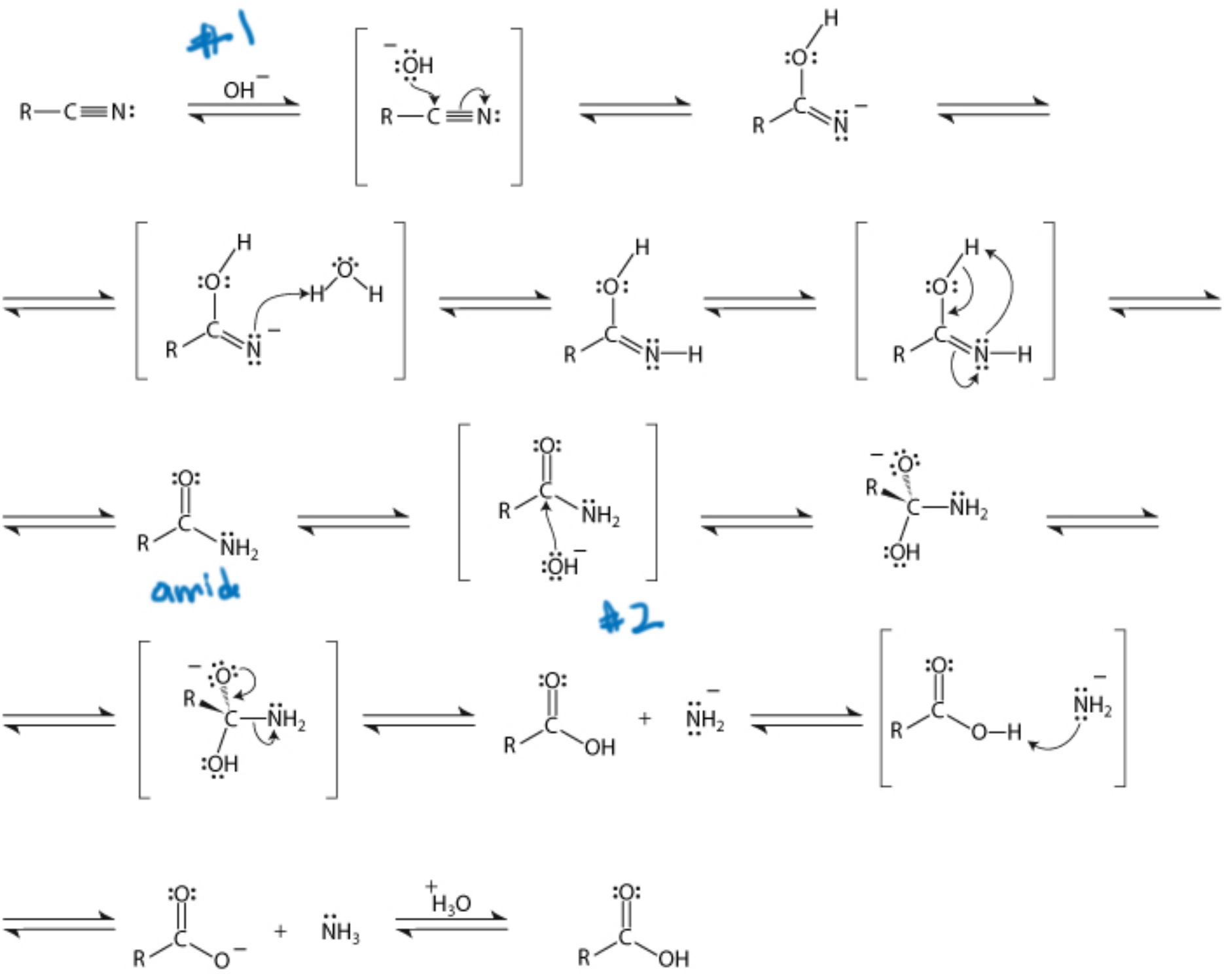


Nitrile

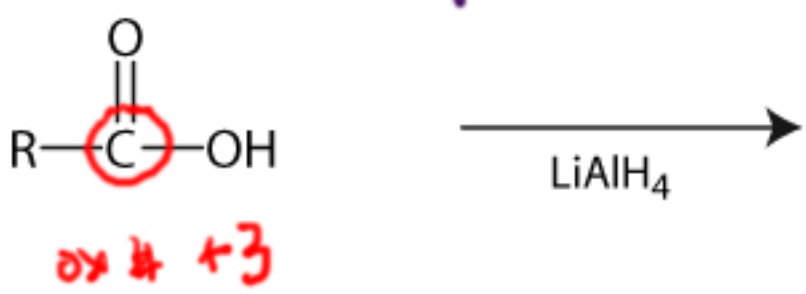
R-C≡N
| 2 H₂O
| (or OH)

R-C(=O)-OH

#1



Reduction of Carboxylic Acid



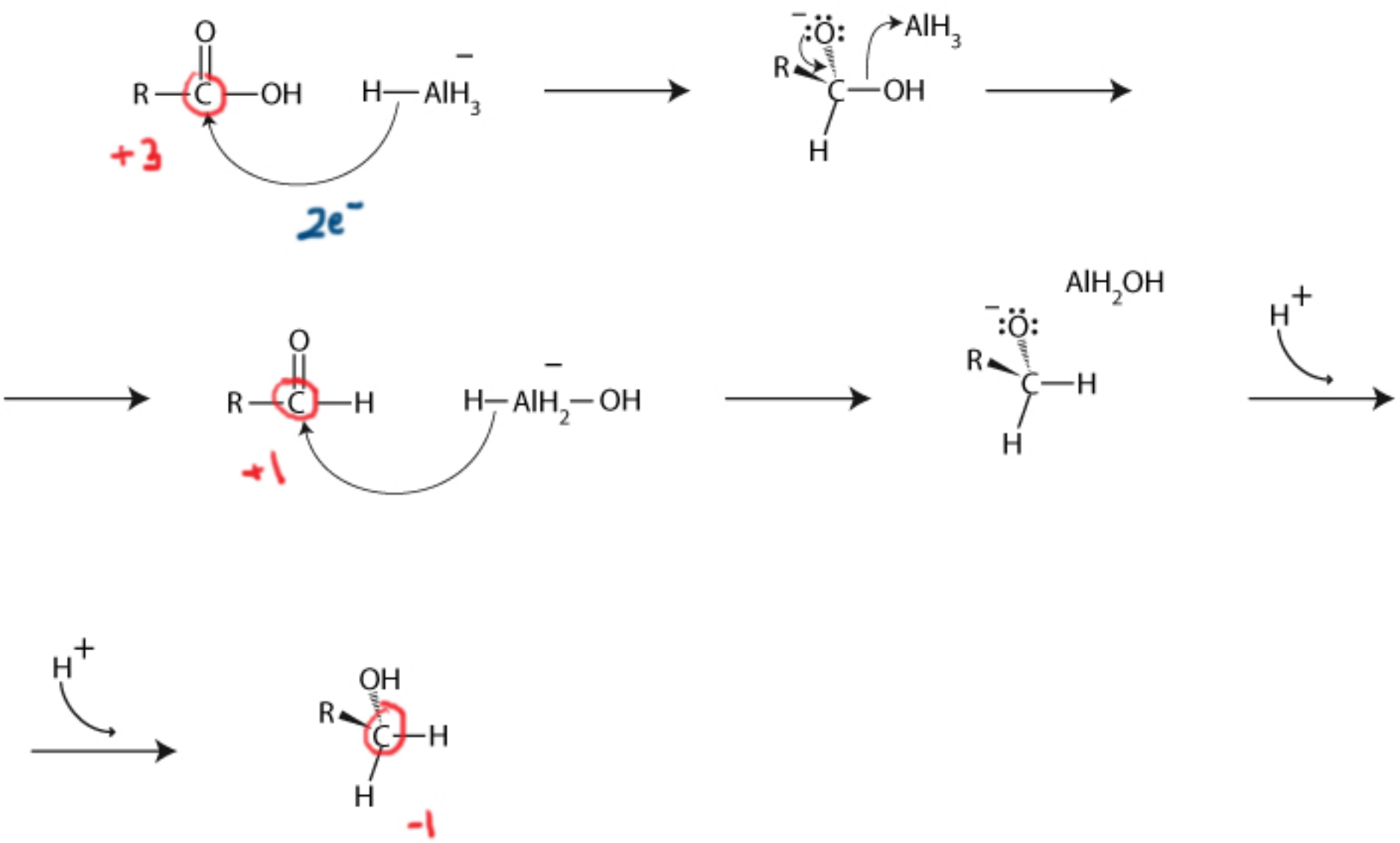
ox # +3

ox # -1

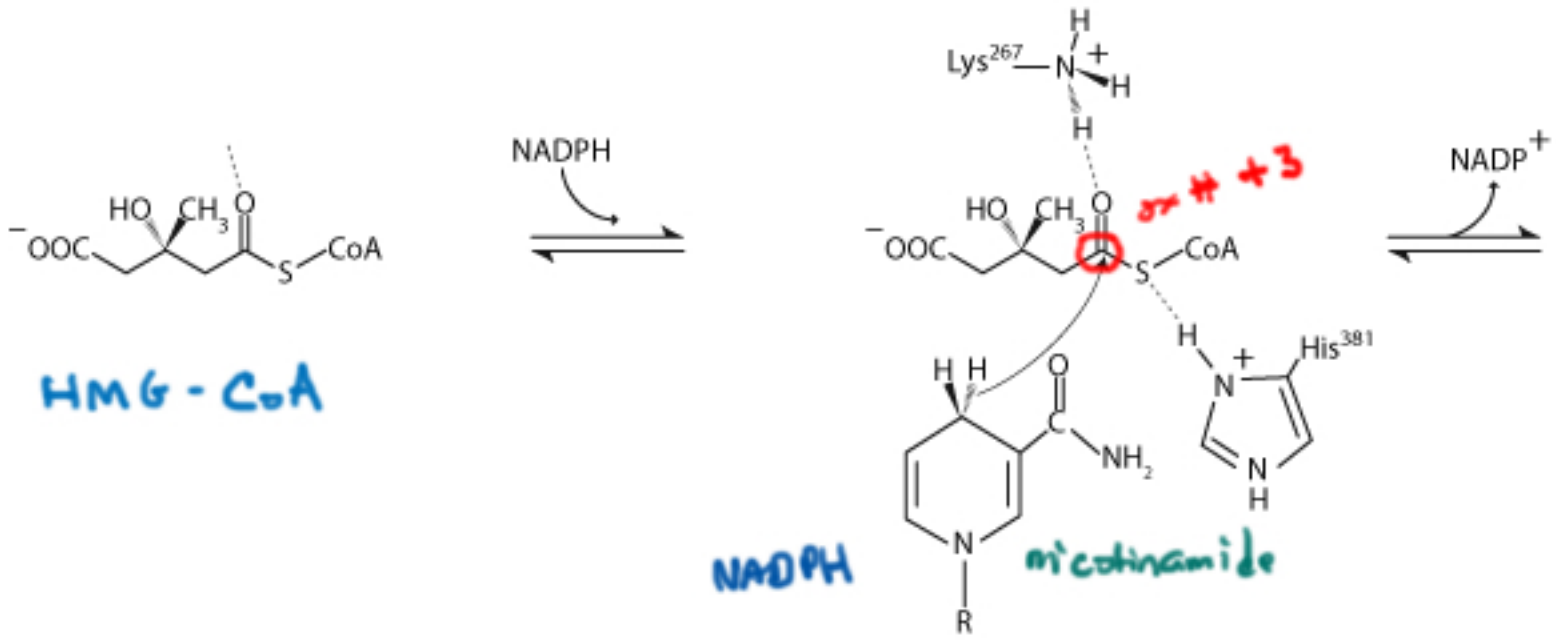
ROH most reduced

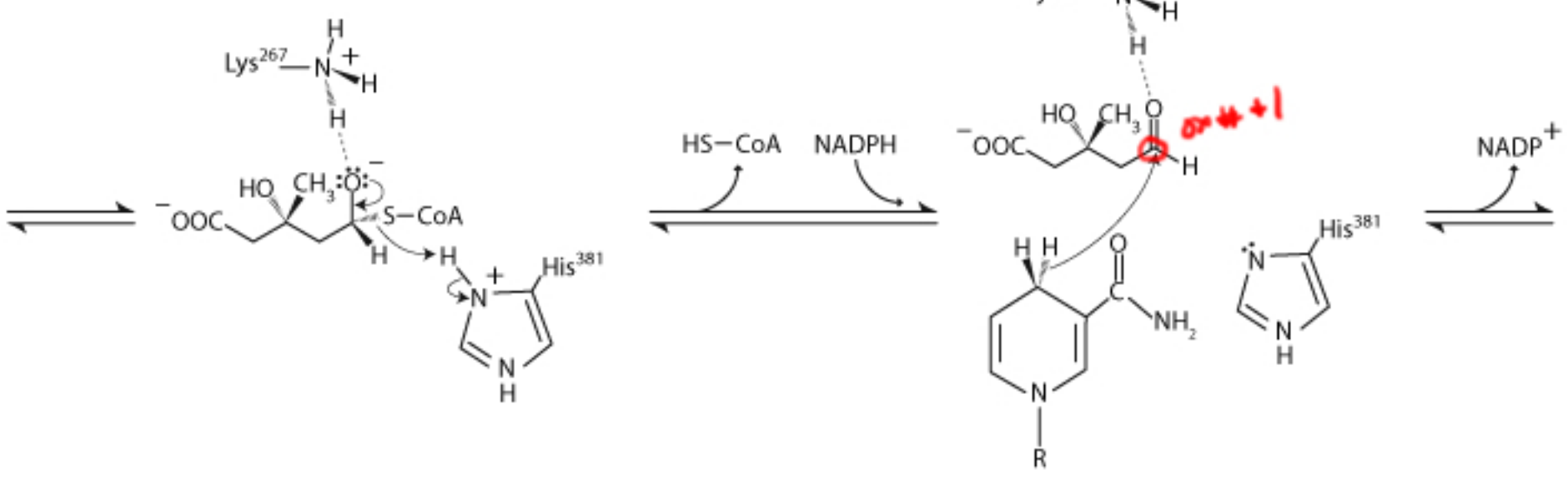
RCH

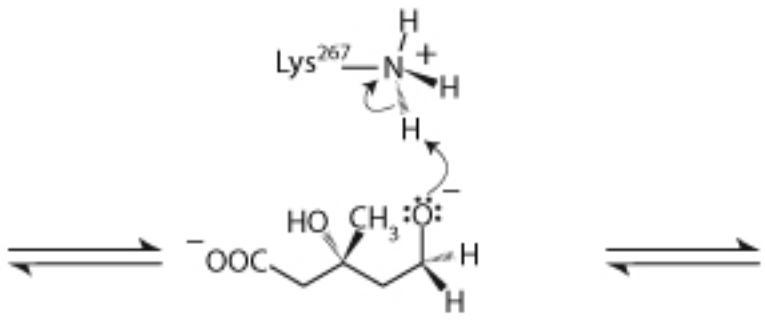
RCOH most oxidized



HMG-CoA Reductase







mevalonate

↓

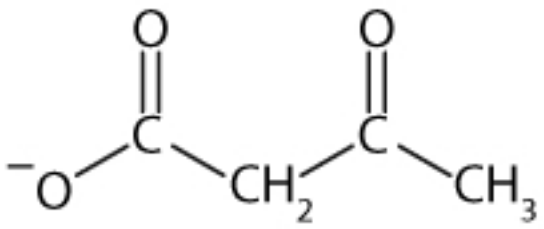
isopentyl pyrophosphate

↓

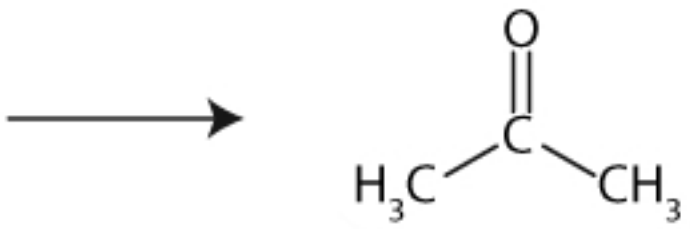
isoprenoid lipids + cholesterol ad steroids

β Keto Acids Decarboxylate Easily

β Keto Acid

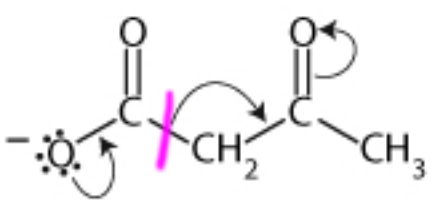


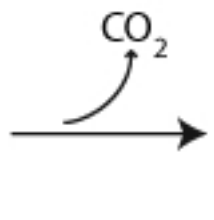
acetoacetate (ketone body)

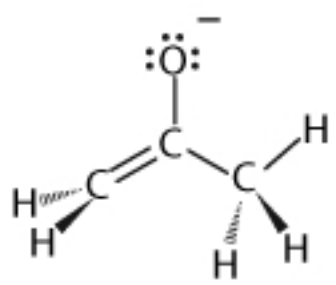


Acetone

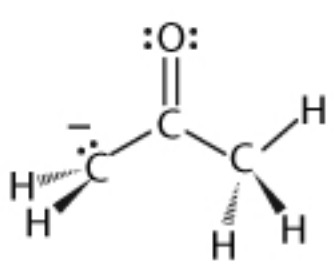
+ CO_2

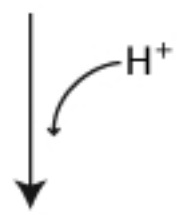


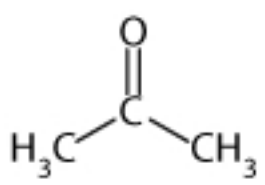


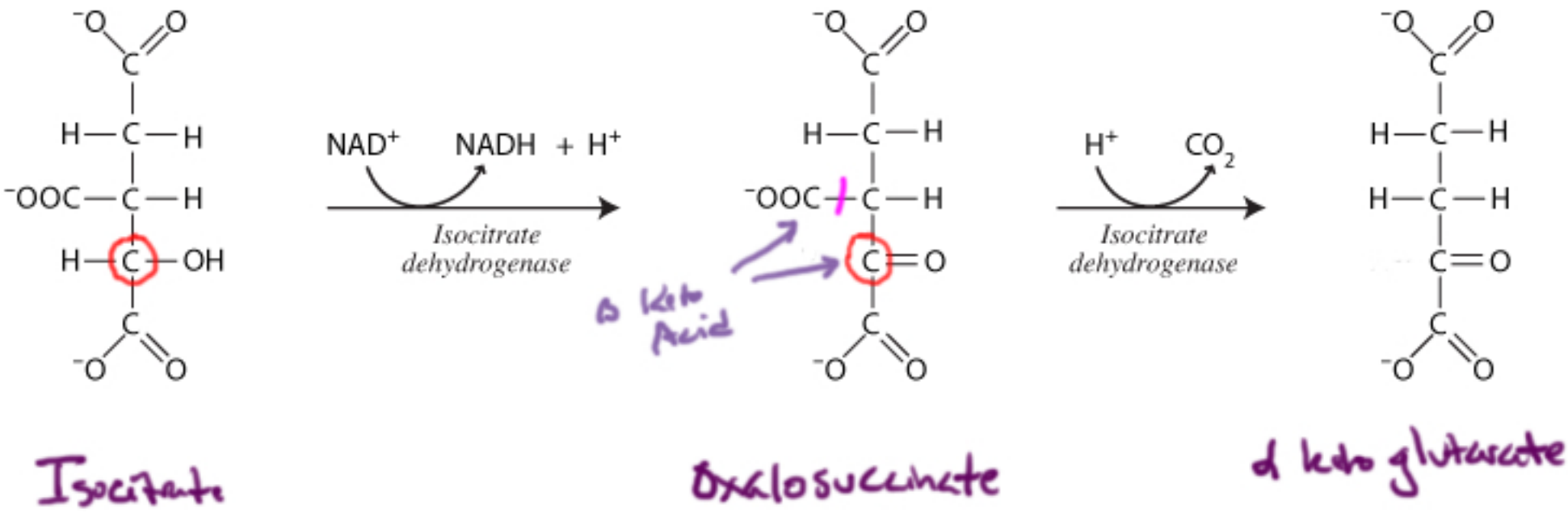


Resonance Stabilized Enolate







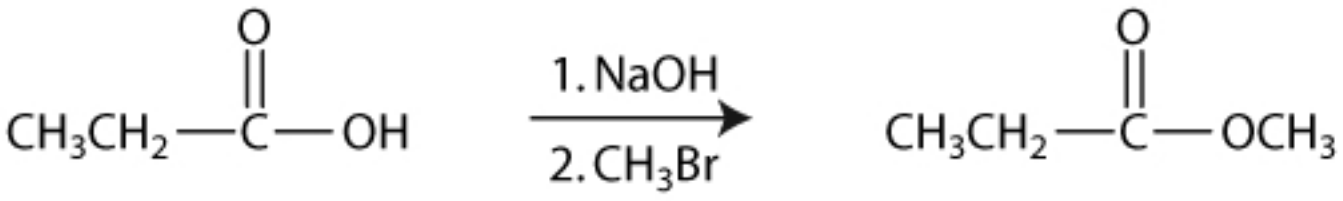


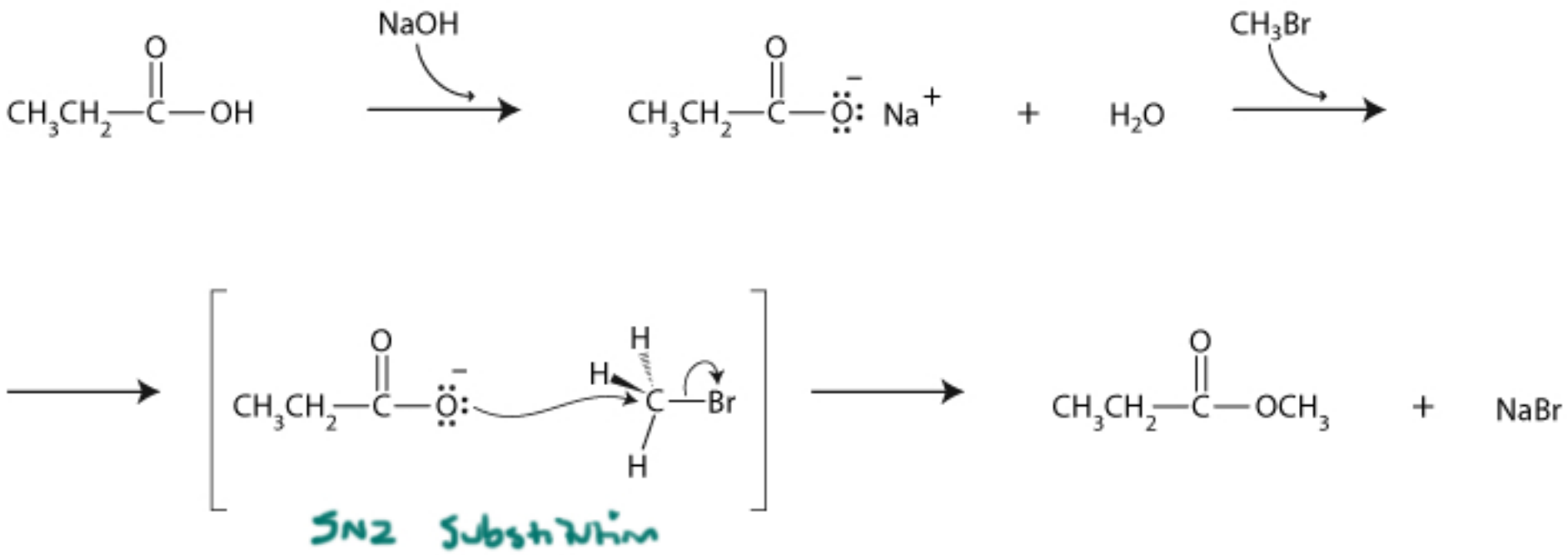
Isocitrate

Oxalosuccinate

α keto glutarate

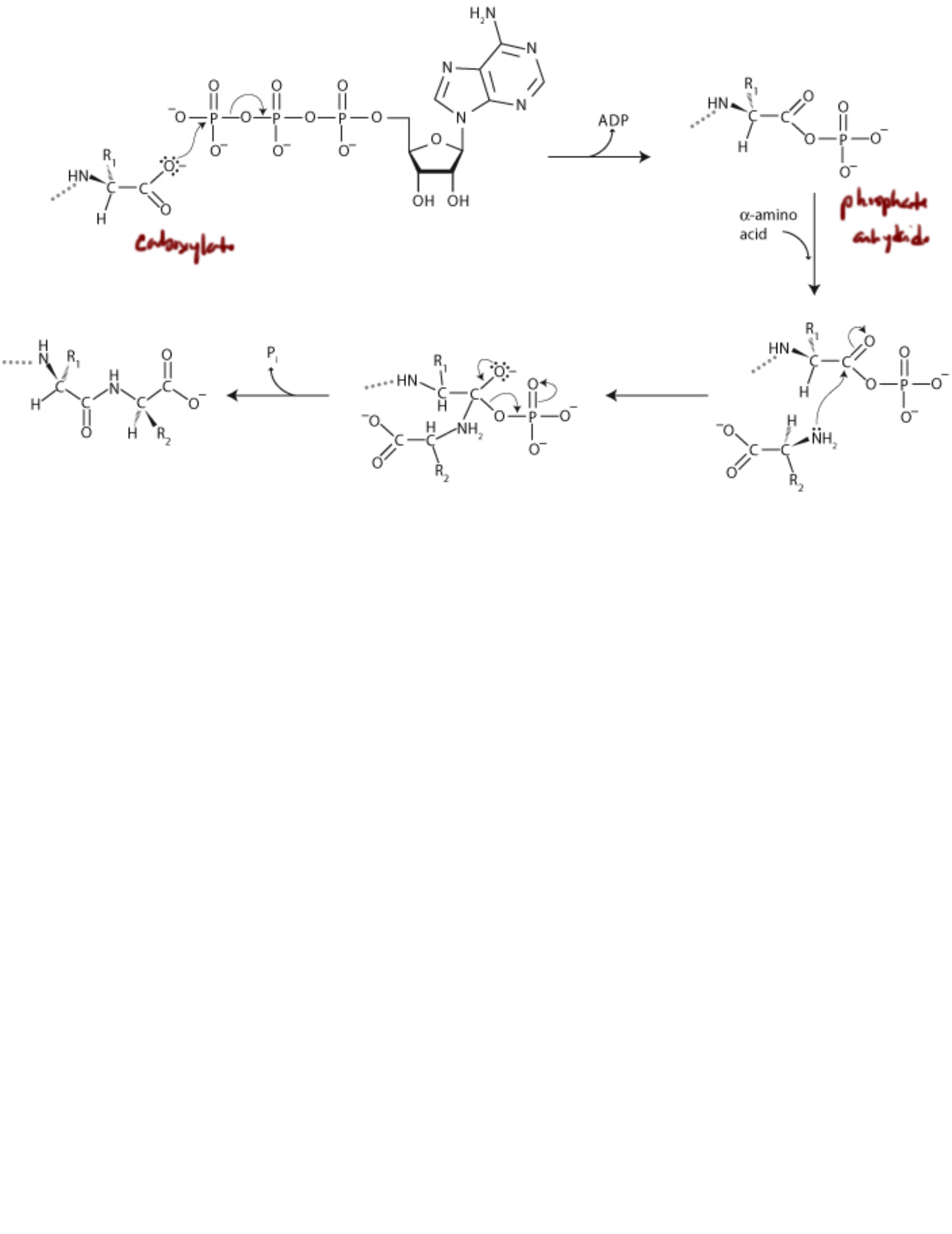
Use of Carboxylate Nucleophile

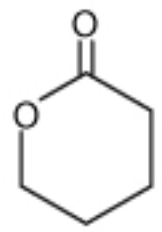




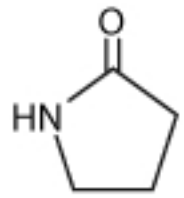
SN2 Substitution

Abiotic Peptide Bond Formation





Lactone



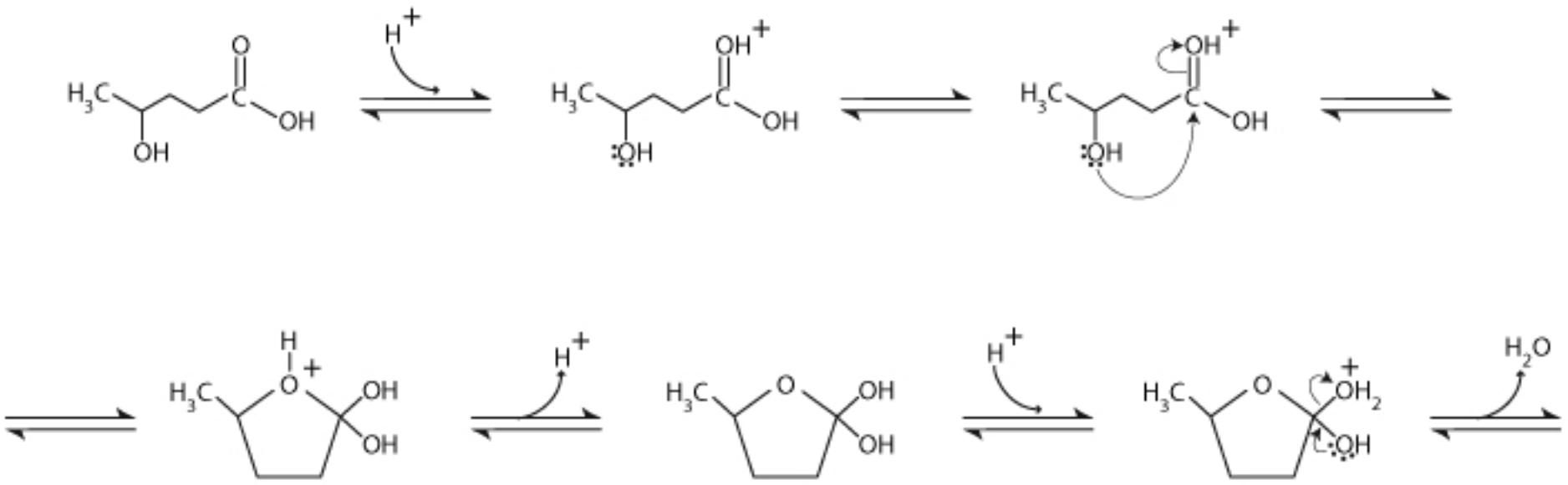
Lactam

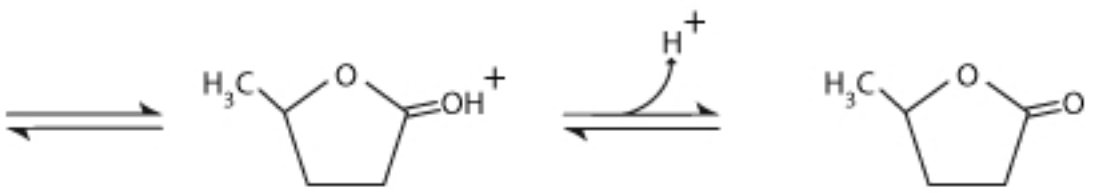
β - 4 membered

γ - 5 membered

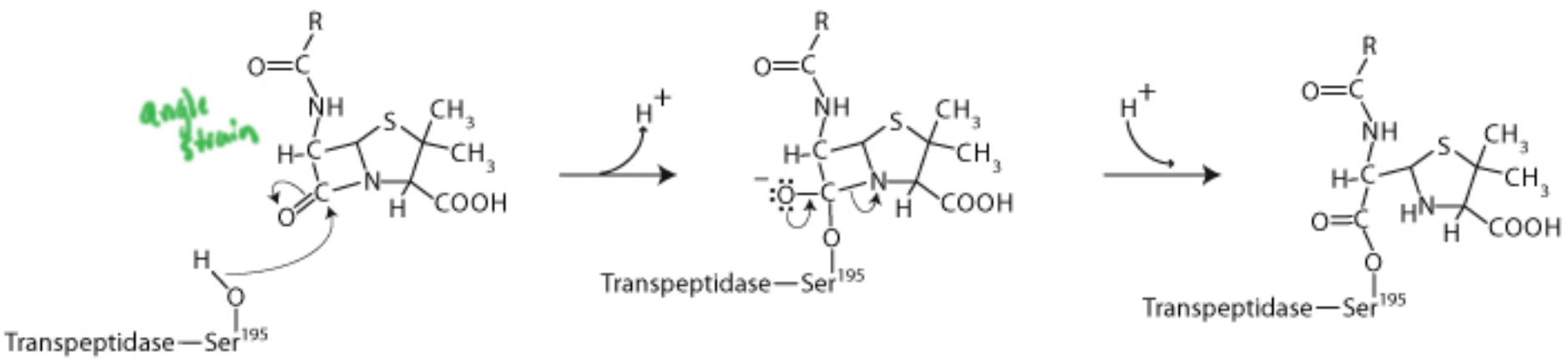
δ - 6 membered

supplemental (Intramolecular acyl substitution)





Penicillin



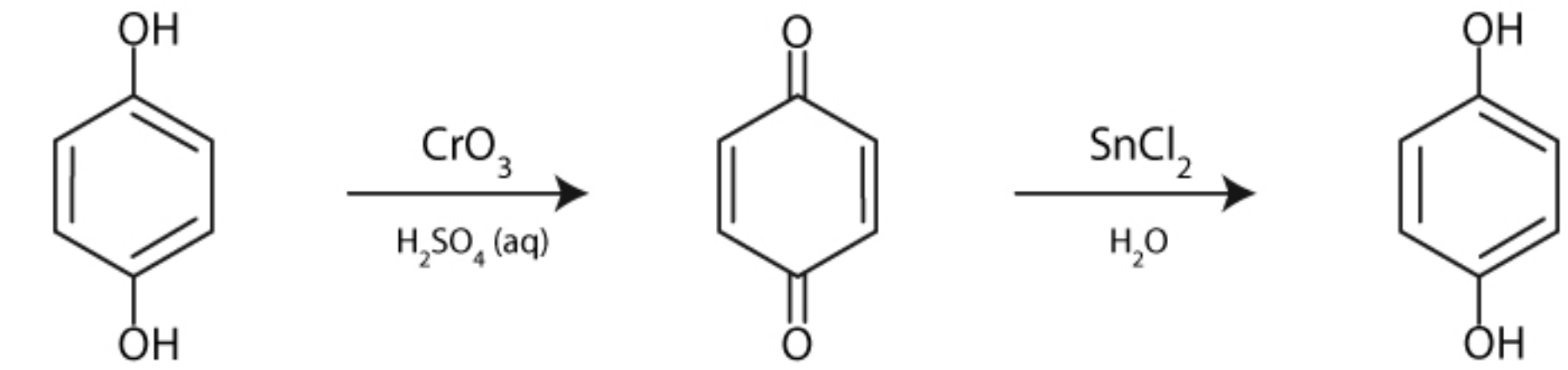
suicide inhibition

Bacterial cell wall -

comprised of peptidoglycan

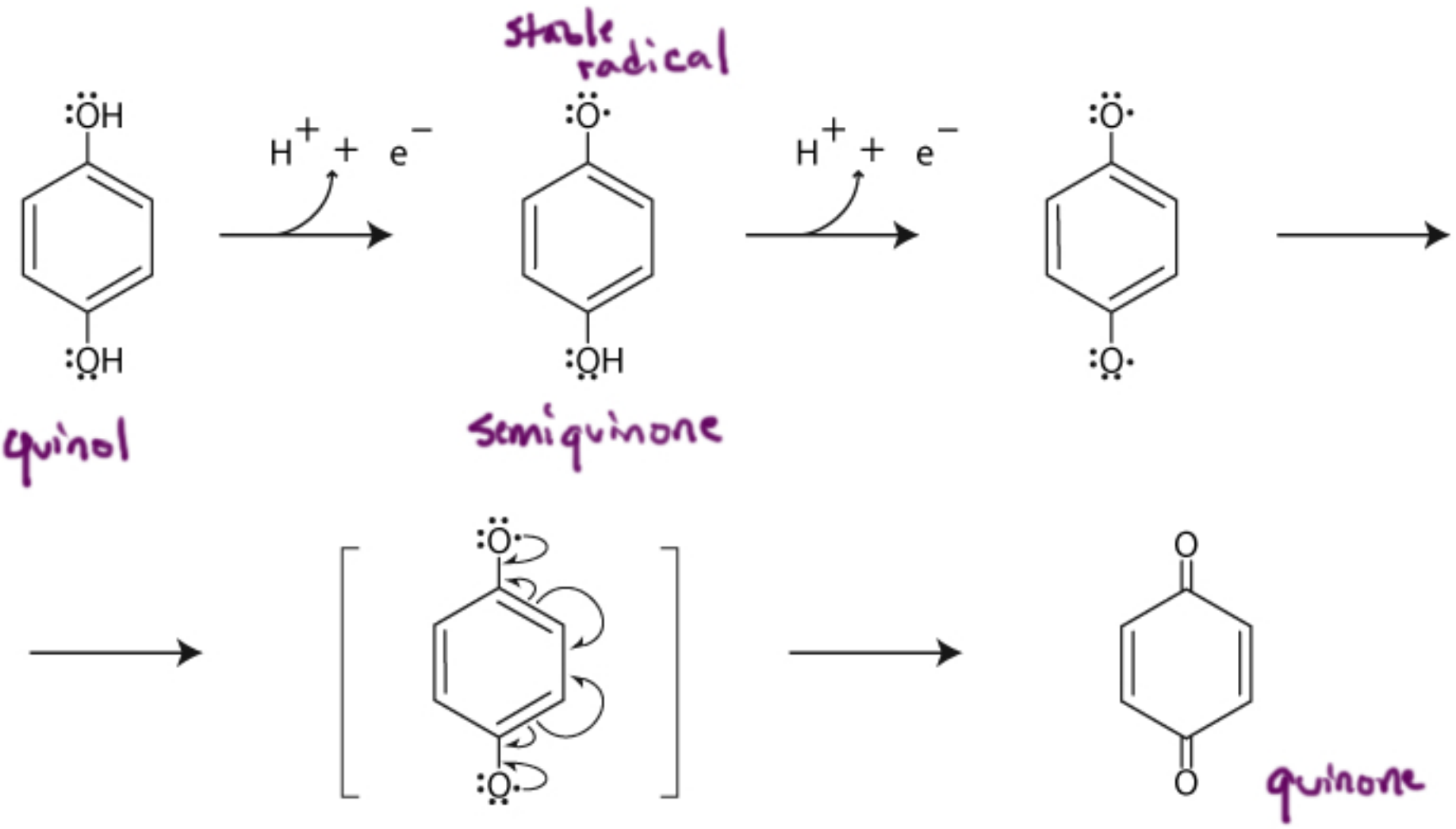
- long chains of NAG (N-acetyl glucosamine)
  NAM (N-acetyl muramic acid)
- with peptide crosslinks formed by transpeptidase

Oxidation of Dihydroxybenzene

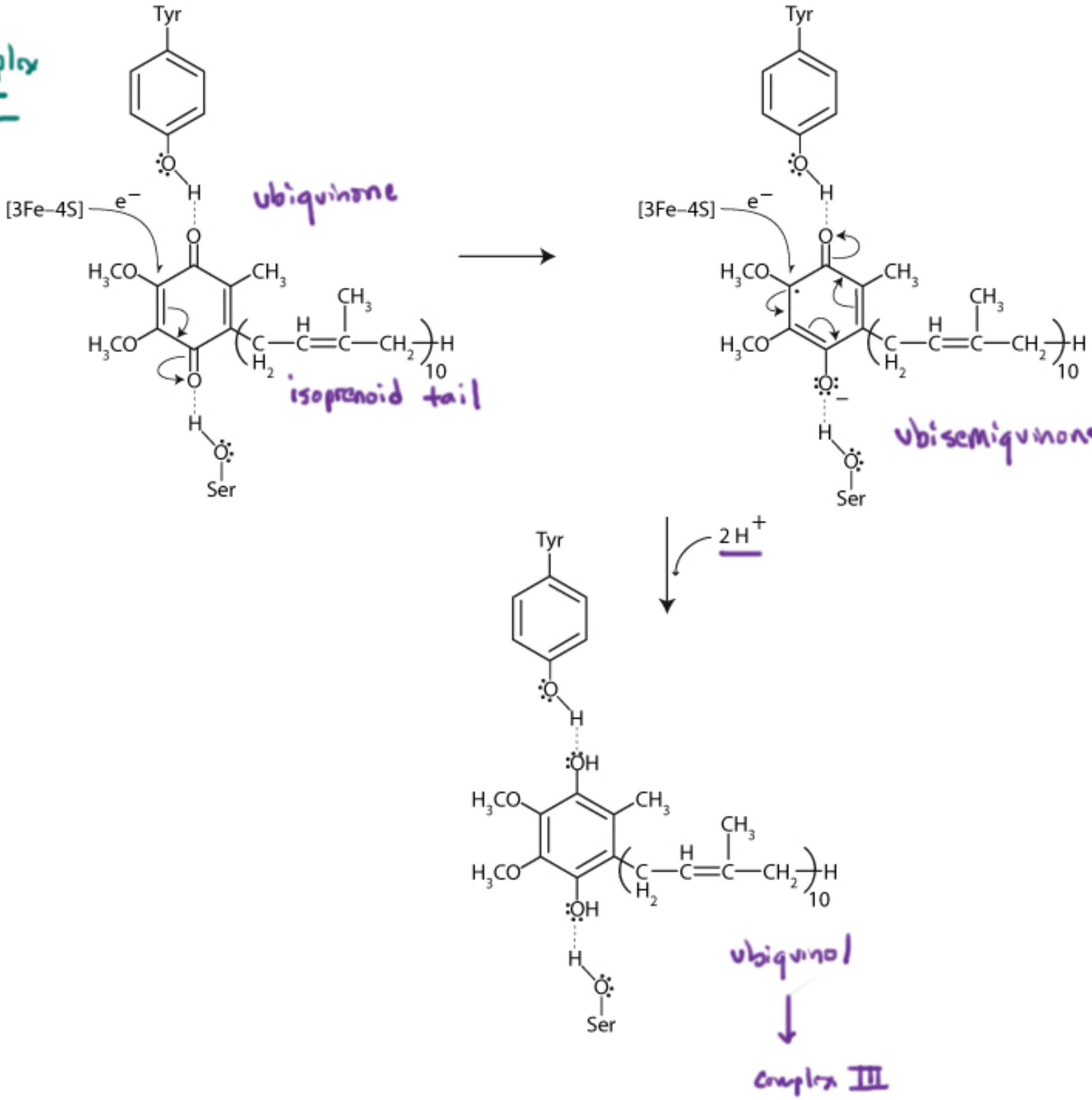


Dihydroxybenzene

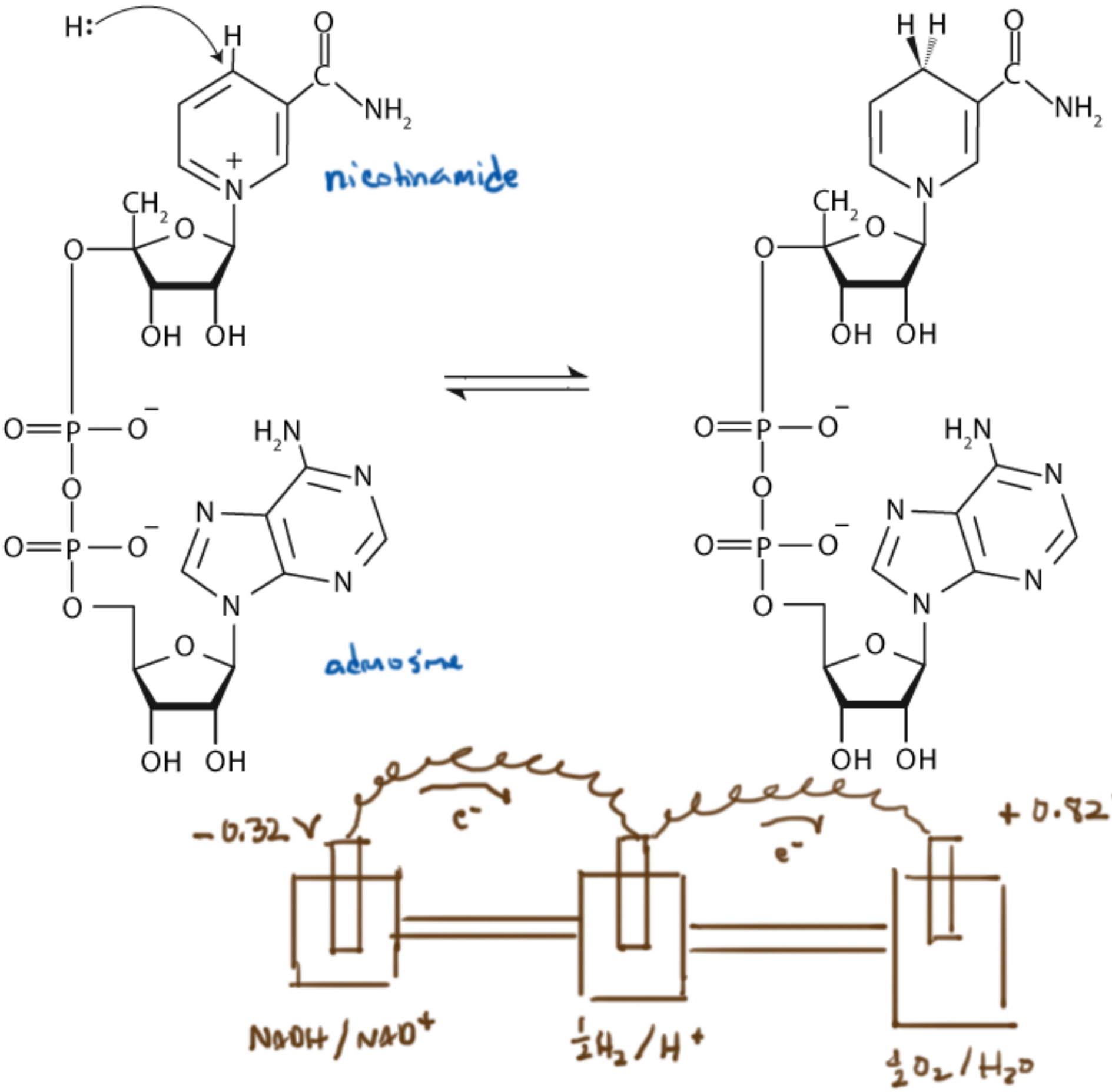
Benzoquinone



Complex II


Tyr
[3Fe–4S]
e⁻
ubiquinone
isoprenoid tail
Ser
ubisemiquinone
2 H⁺
ubiquinol
Complex III

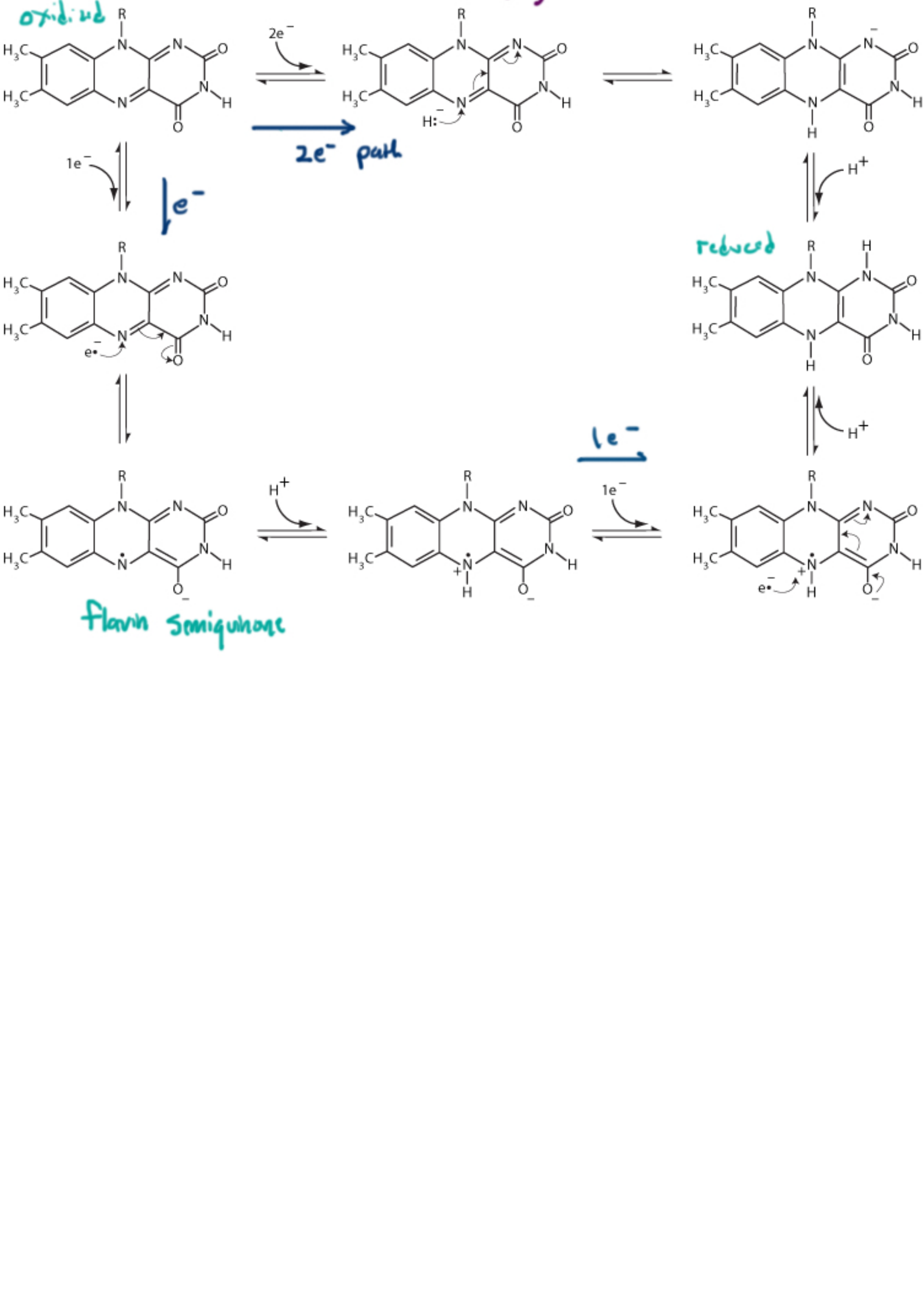
Reduction of NADH



$$E_{cell} = E^{\circ}_{cathode} - E^{\circ}_{anode}$$

$$= 0.92\,V - (-0.32\,V) = 1.14\,V$$

Flavin (isoNoxazine ring)



Molecular spectroscopy

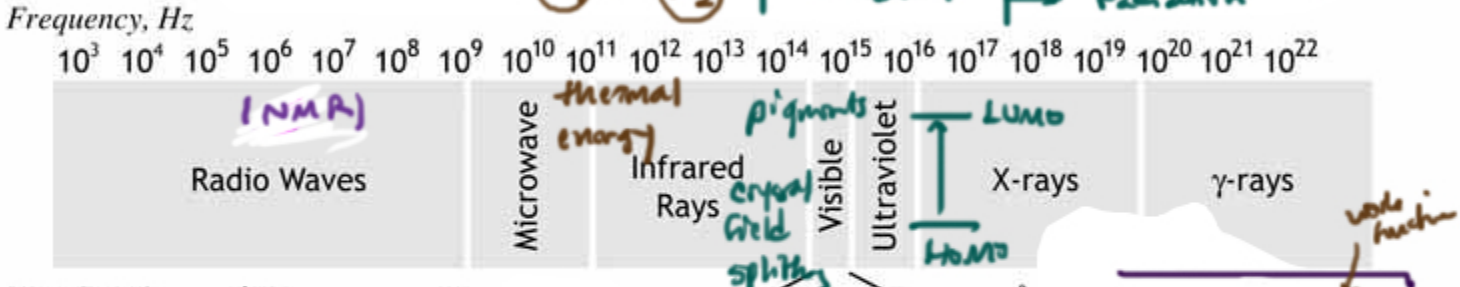
IR

$f = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$

$\mu = \frac{m_1 m_2}{m_1 + m_2}$

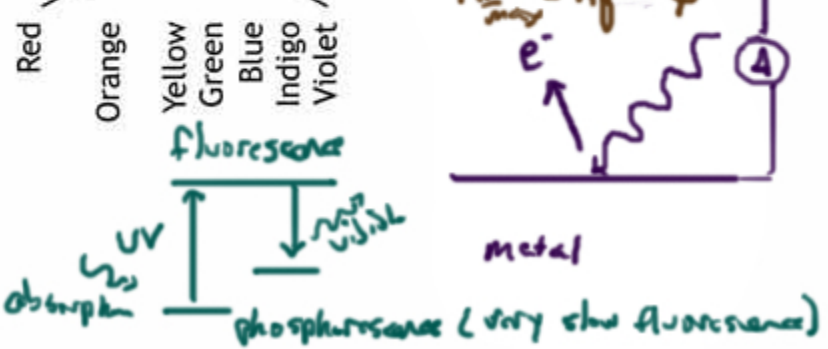
$E = hf$

electronic transition → ionising radiation

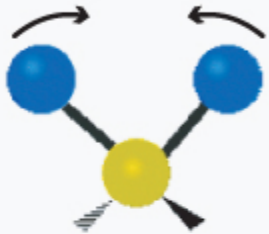
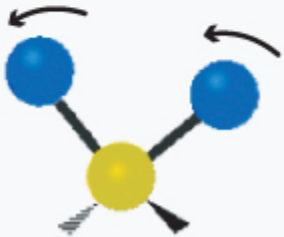
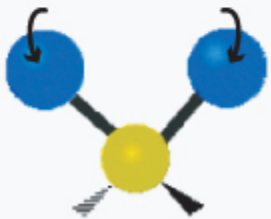
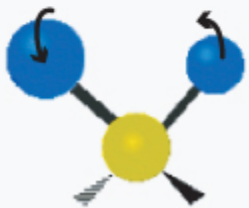


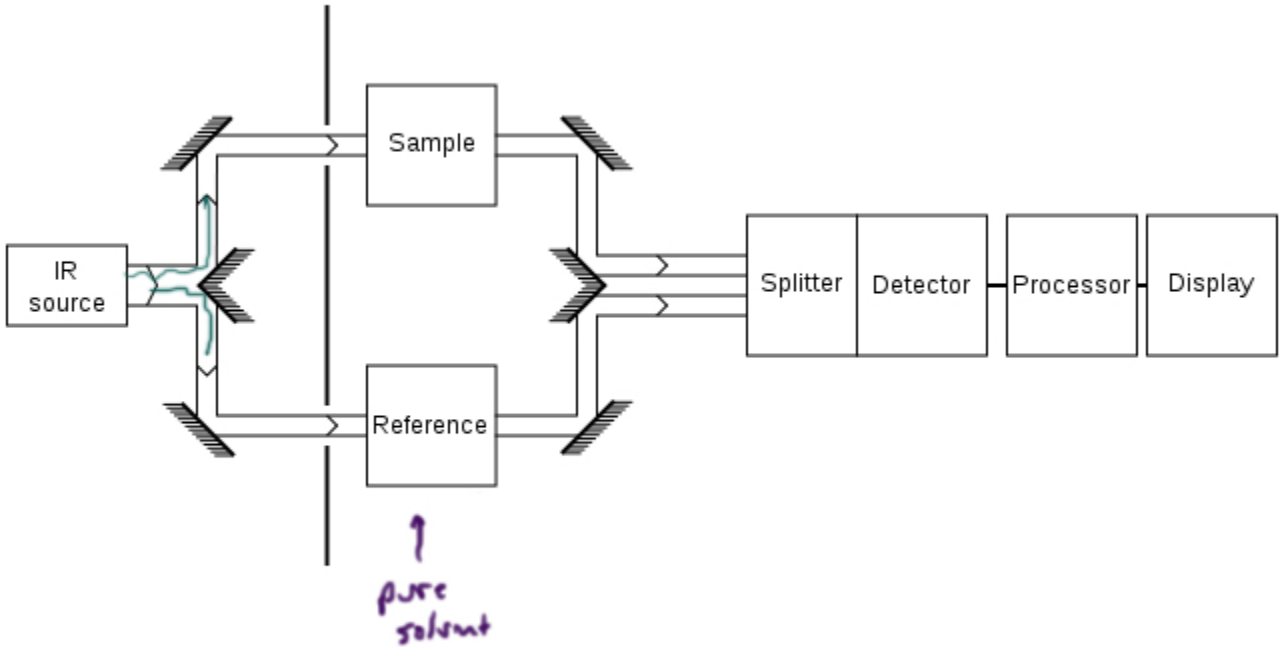
$1\ eV = 1.6 \times 10^{-19}\ J$

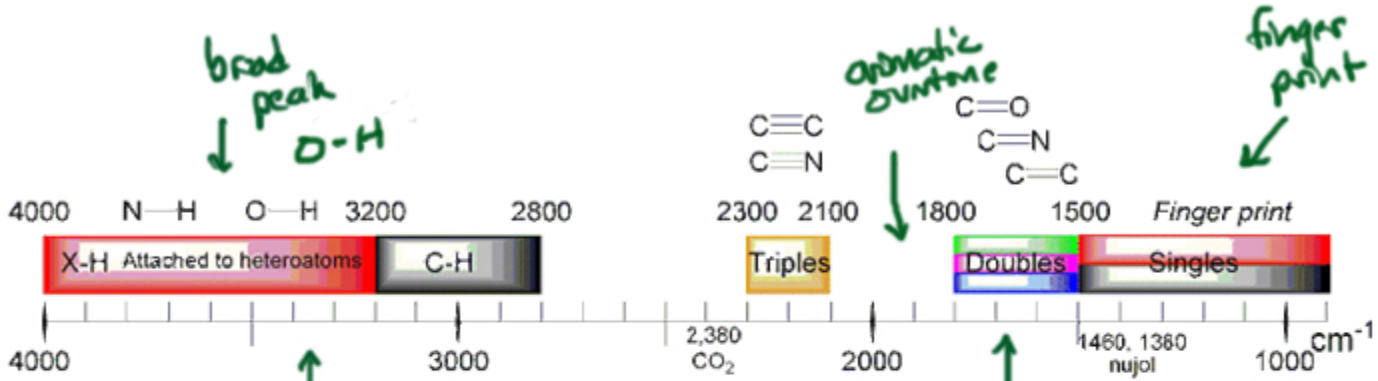
the world LV does on 1e



IR spec

Symmetric stretching	Antisymmetric stretching	Scissoring
		
Rocking	**Wagging**	**Twisting**
		


Sample
IR source
Reference
Splitter
Detector
Processor
Display
pure solvent



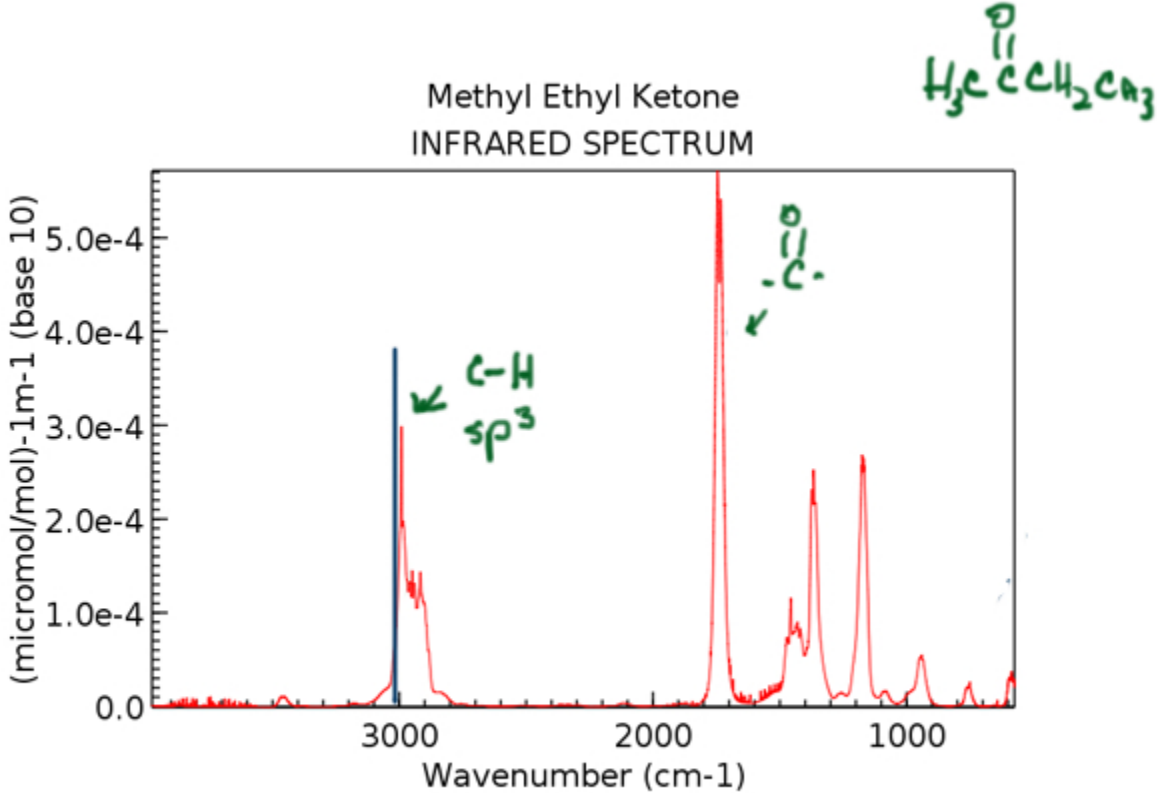
$$\tilde{\nu} = \frac{1}{\lambda}$$

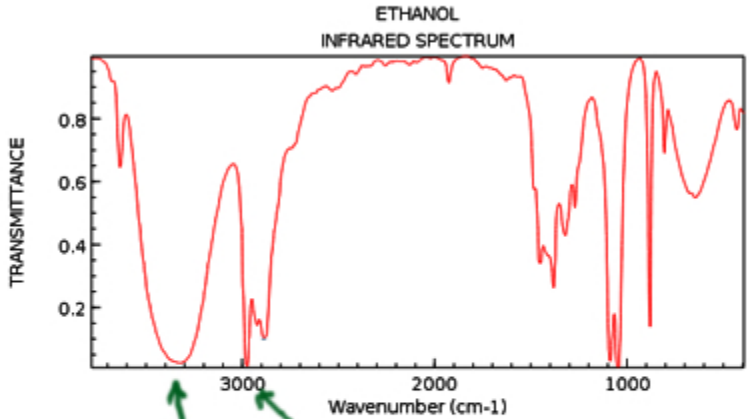
cm^{-1} - $\frac{\text{cycles}}{cm}$

spatial frequency

$V = f\lambda$ $\quad f = \frac{1}{\lambda} V$

> 3000
C-H stretch
sp^2
vinylic, or aromatic

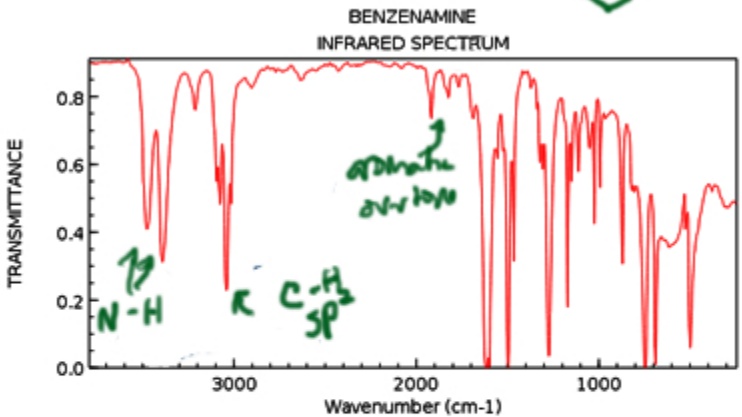

Methyl Ethyl Ketone
INFRARED SPECTRUM
(micromol/mol)-1m-1 (base 10)
5.0e-4
4.0e-4
3.0e-4
2.0e-4
1.0e-4
0.0
3000
2000
1000
Wavenumber (cm-1)
C-H
sp3
O
C
H3C C CH2 CH3



O-H

C-H
sp^3

Could sharpen by diluting the sample

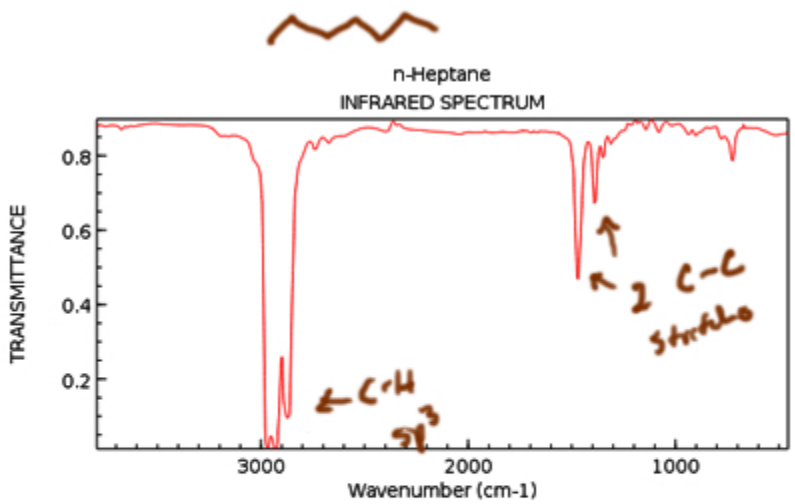


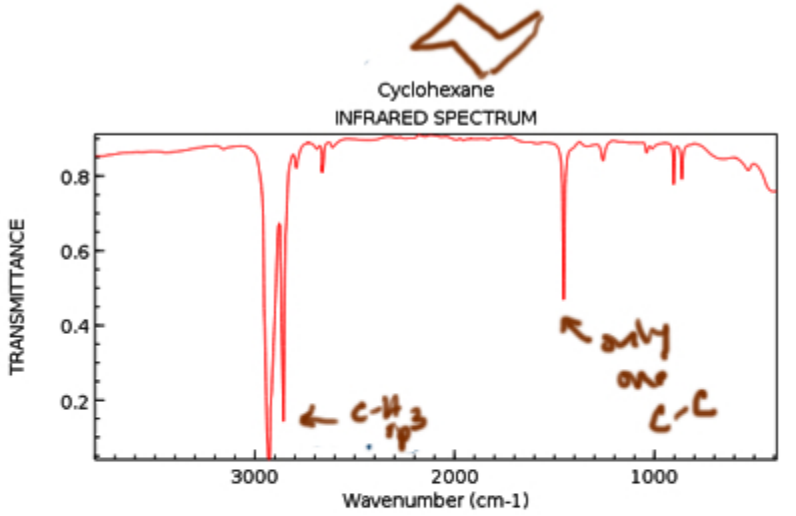
NH_2

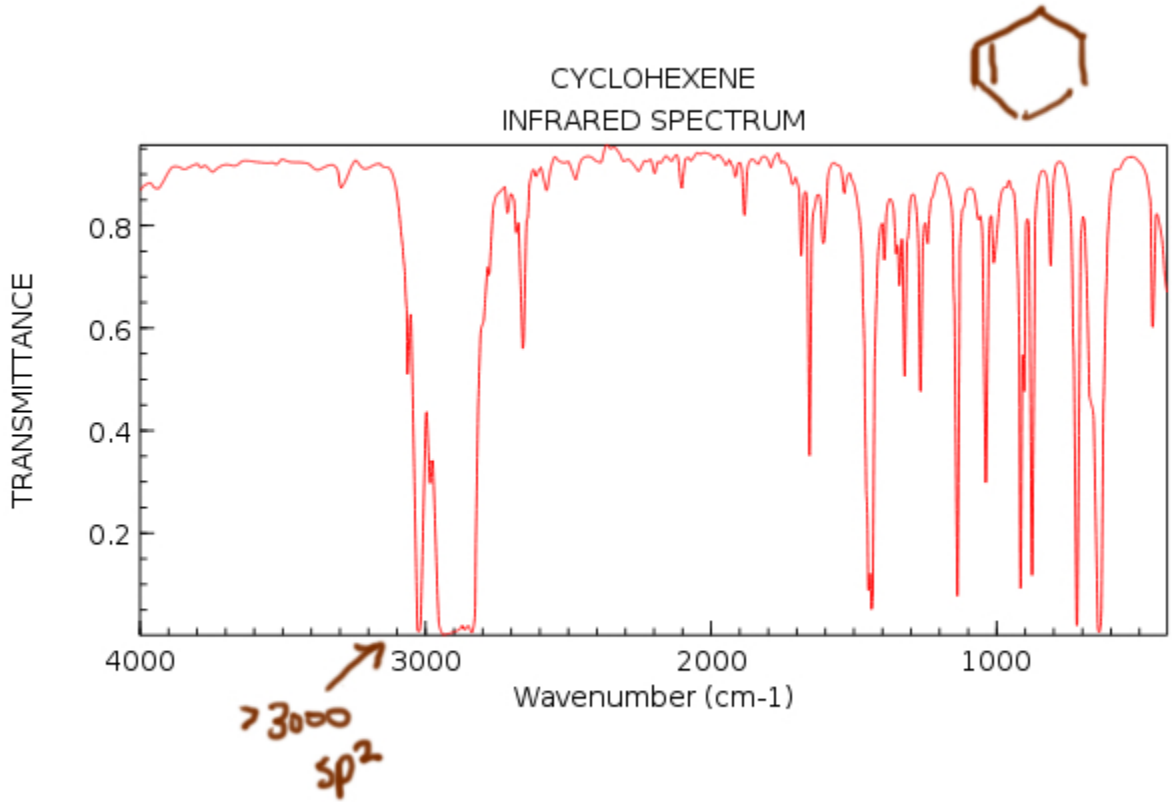
aromatic overtone

N-H

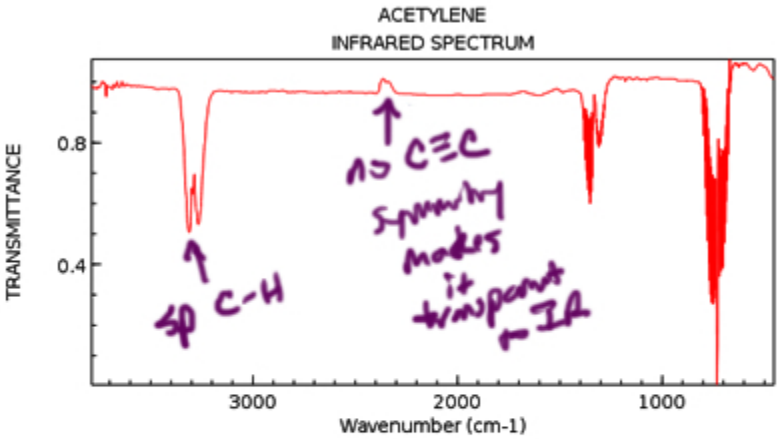
C-H
sp^2


n-Heptane
INFRARED SPECTRUM
TRANSMITTANCE
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)
C-H
sp3
2 C-C
stretch

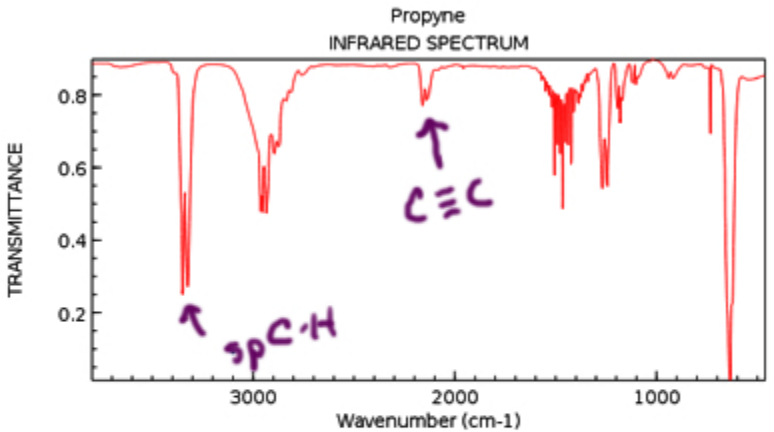

Cyclohexane
INFRARED SPECTRUM
TRANSMITTANCE
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)
C-H
sp3
only
one
C-C

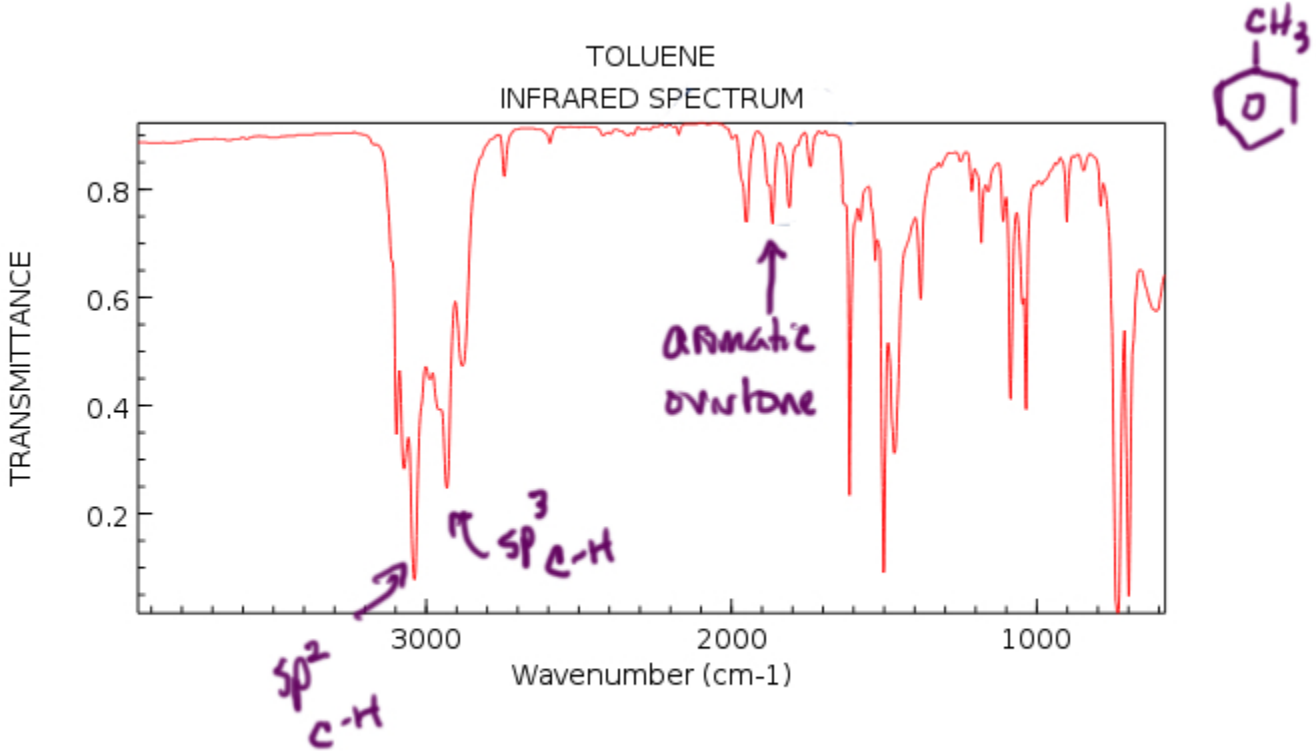

CYCLOHEXENE
INFRARED SPECTRUM
TRANSMITTANCE
0.8
0.6
0.4
0.2
4000
3000
2000
1000
Wavenumber (cm-1)
>3000
sp2

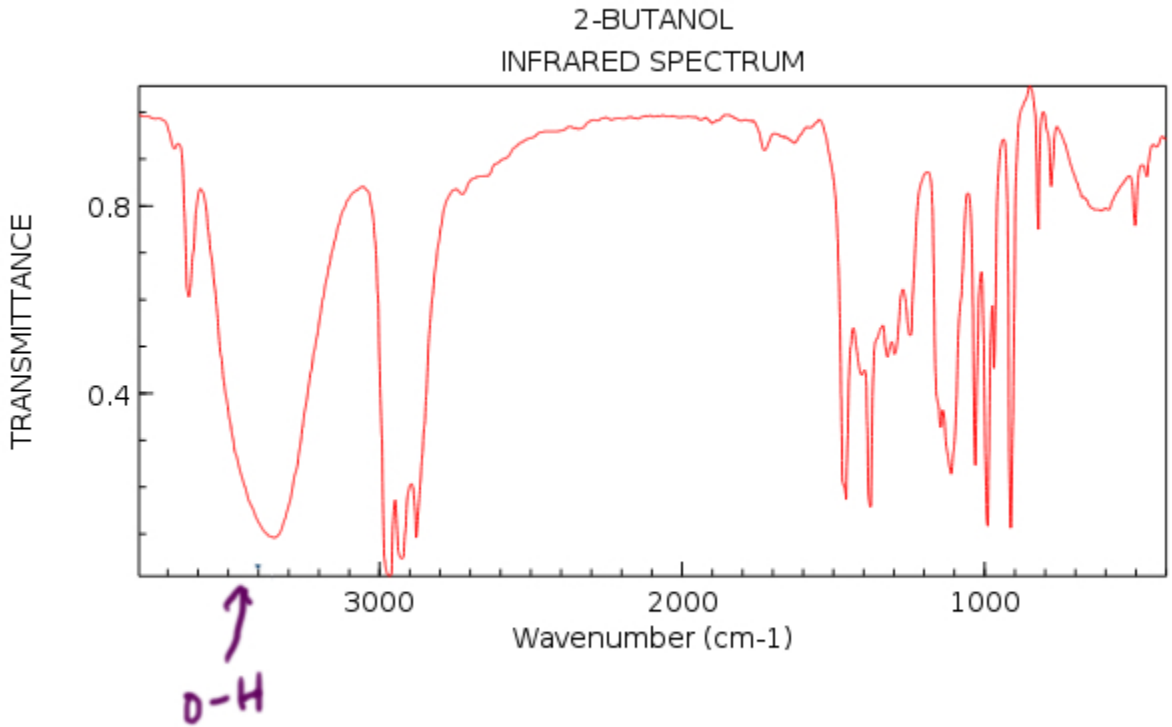
$HC \equiv CH$

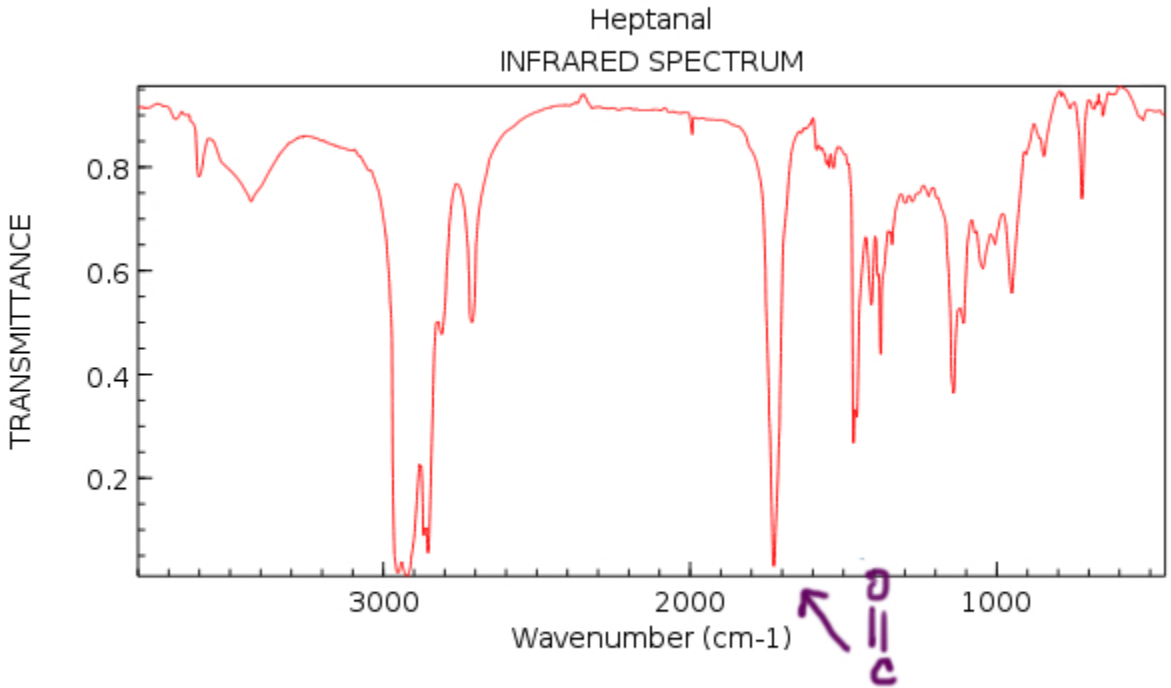


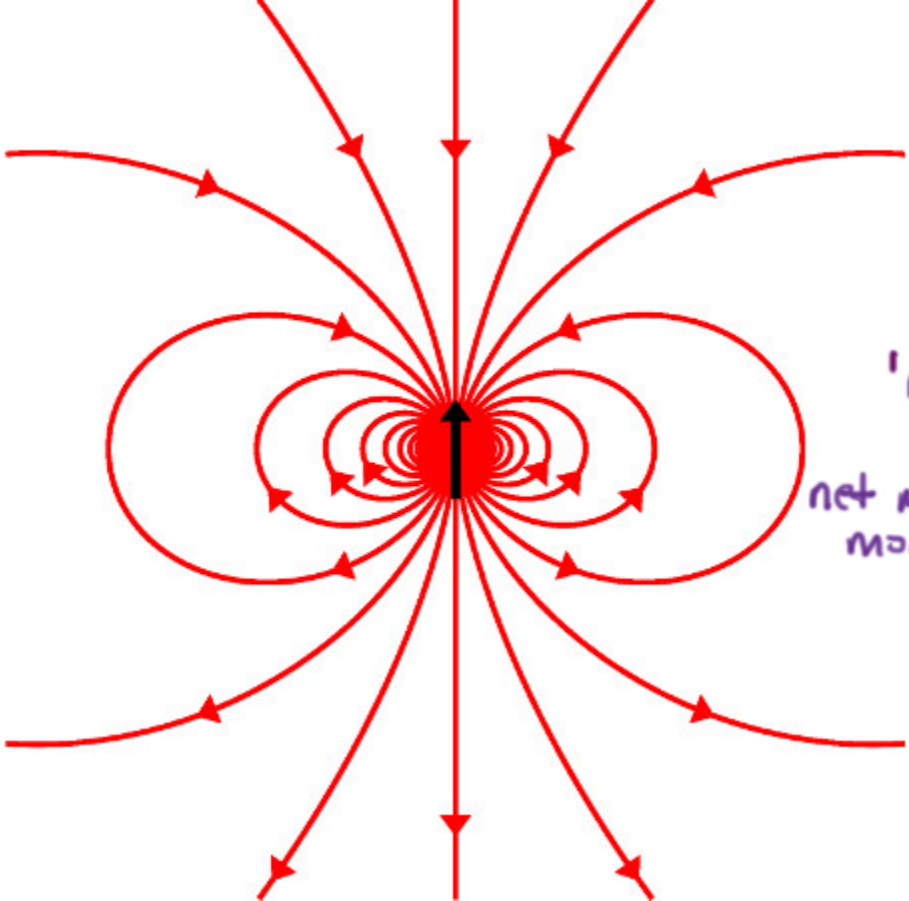
$HC \equiv C-CH_3$

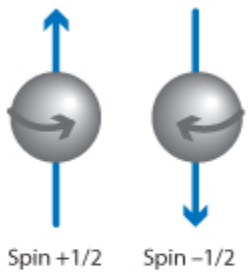



TOLUENE
INFRARED SPECTRUM
TRANSMITTANCE
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)
aromatic overtone
sp3 C-H
sp2 C-H
CH3

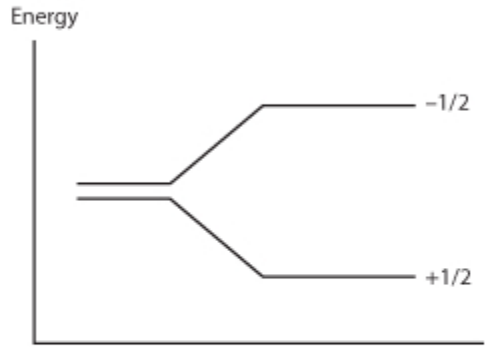

2-BUTANOL
INFRARED SPECTRUM
TRANSMITTANCE
0.8
0.4
3000
2000
1000
Wavenumber (cm-1)
O-H


Heptanal
INFRARED SPECTRUM
TRANSMITTANCE
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)
O
C


^{1}H NMR
^{1}H
net magnetic moment

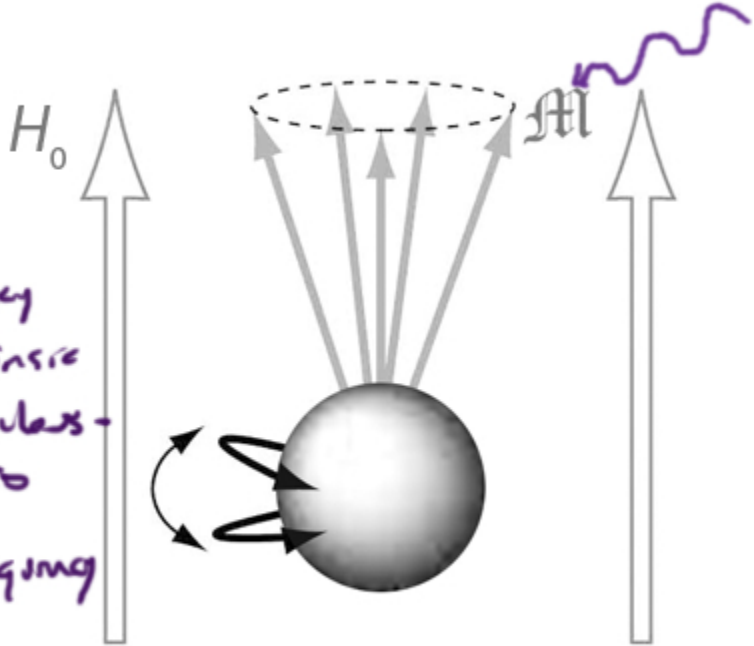


external magnetic field



energy difference in applied field

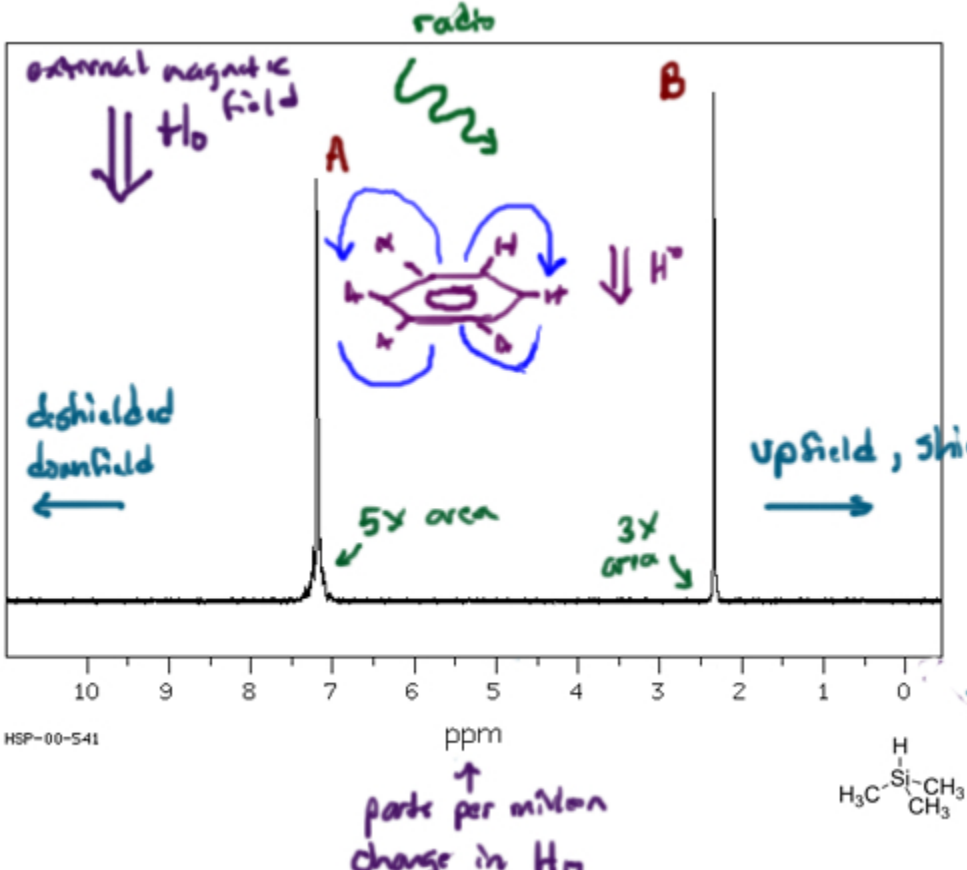
A nuclear spin precesses around an external field

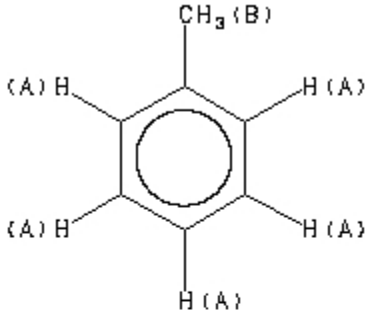


Precessional frequency depends on an intrinsic property of the nucleus - gyromagnetic ratio

- Precessional frequency increases with external field

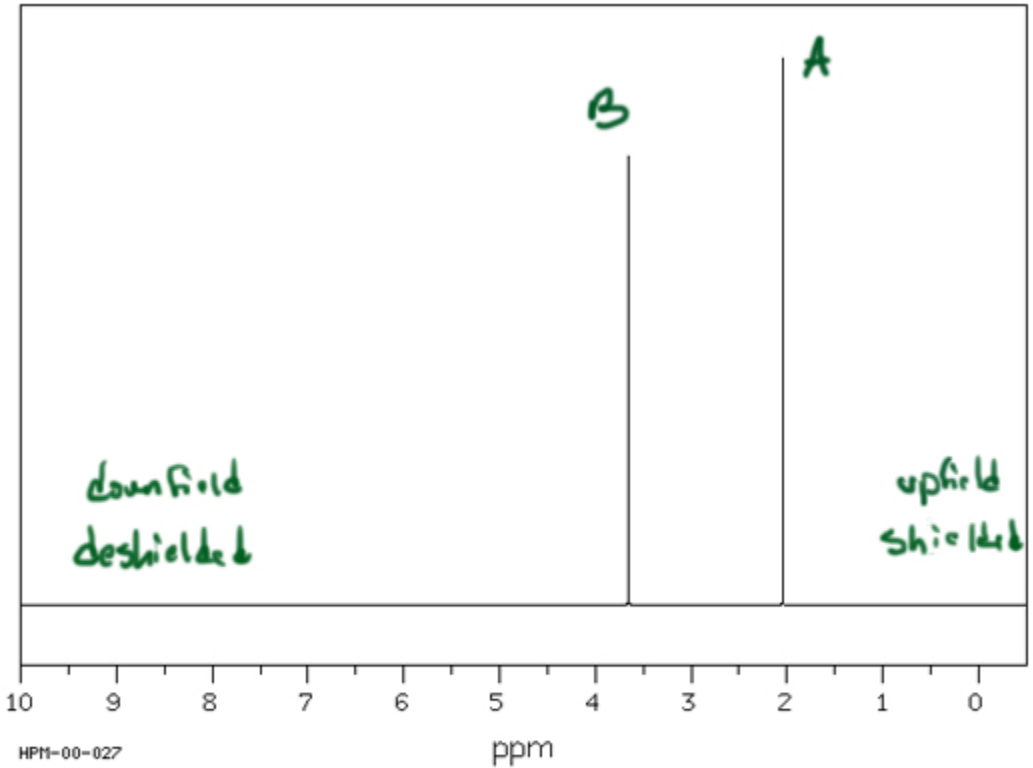
Resonance occurs when incident radio waves are the same as the precessional frequency.



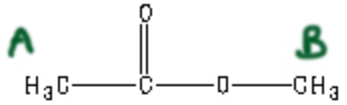


very very shielded

← TMS



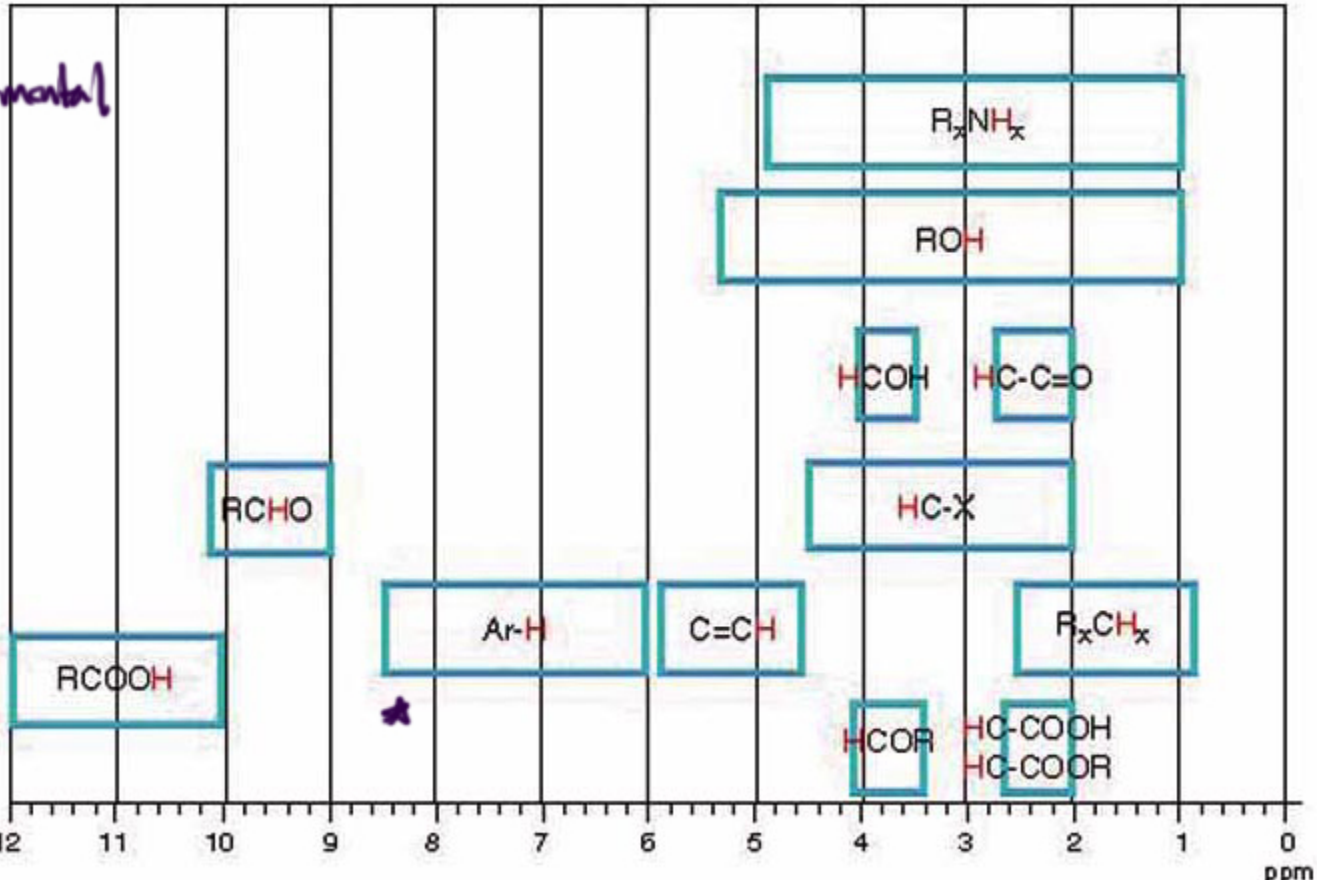
← Subtracting ppm from H_o

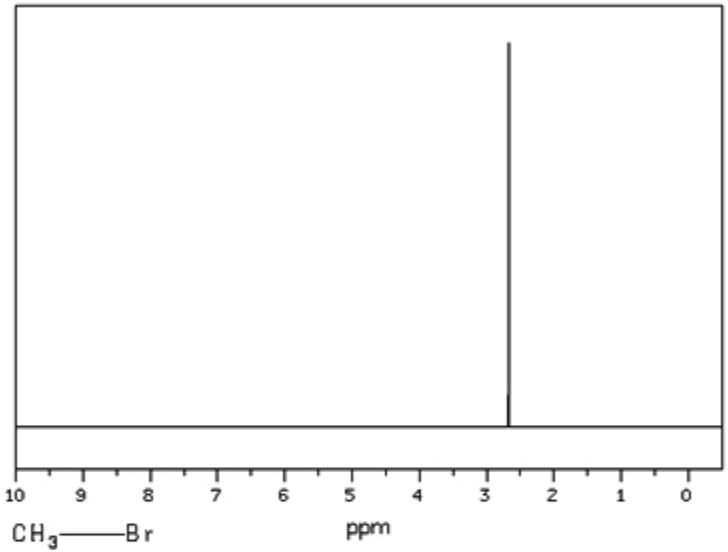


↑

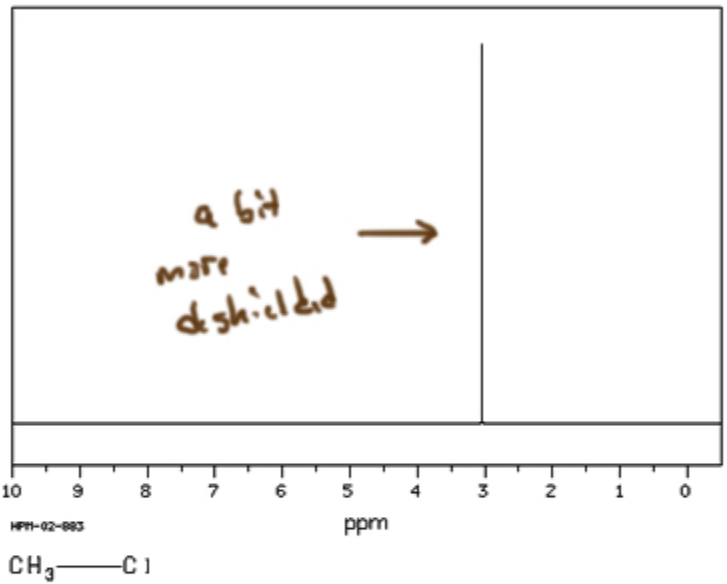
deshielded by oxygen and shifted downfield

Supplemental

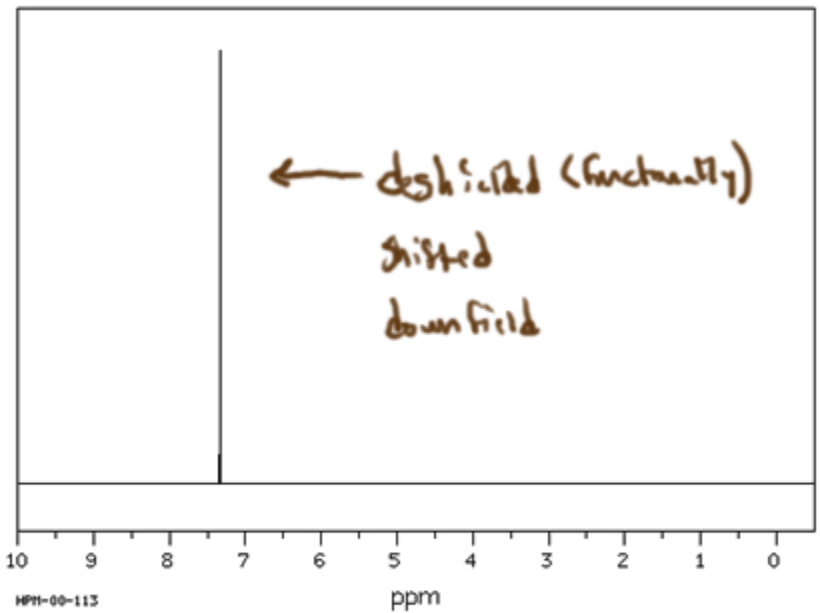


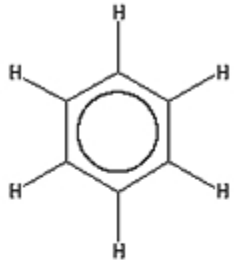


Br electronegativity 2.8

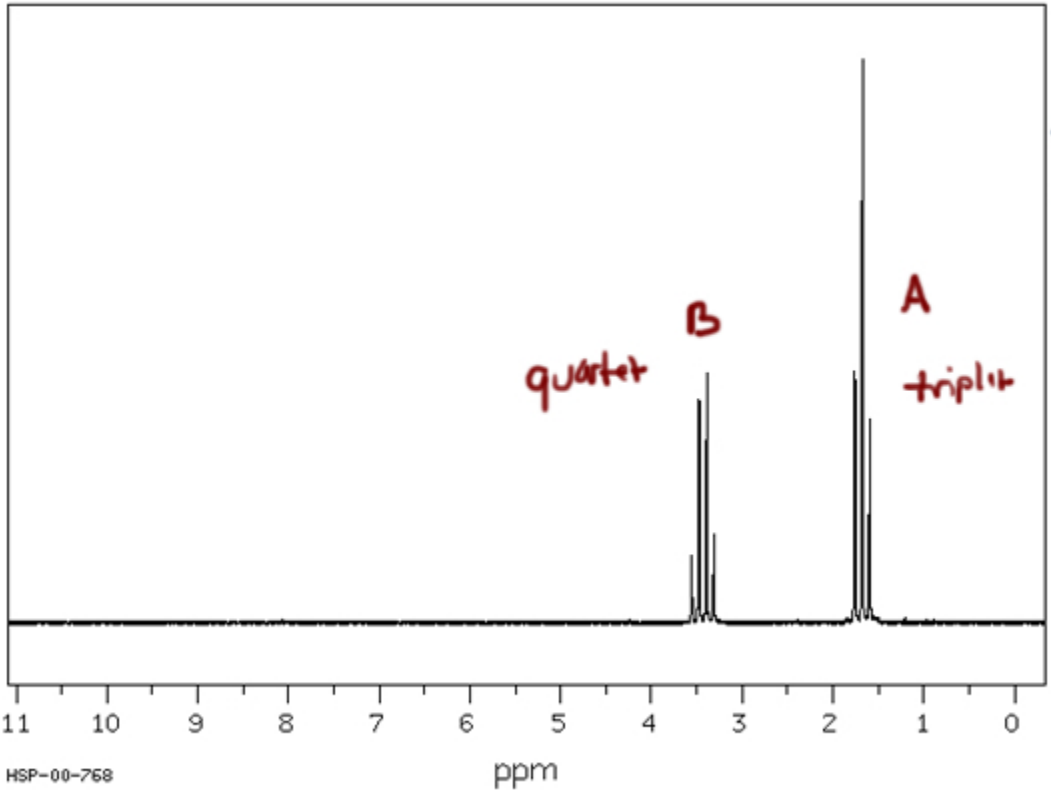


Cl electronegativity 3.0


← deshielded (fractionally)
shifted
downfield
10
9
8
7
6
5
4
3
2
1
0
ppm
HPH-00-113


H
H
H
H
H
H

ring current
field
reinforces
the external
field
H
H
H
H
H
H
H₀



A B

$CH_3—CH_2—Br$

these affect the shielding of those

deshielding

shielding

↑↑↑ ↑↑↓ ↓↓↑ ↓↓↓

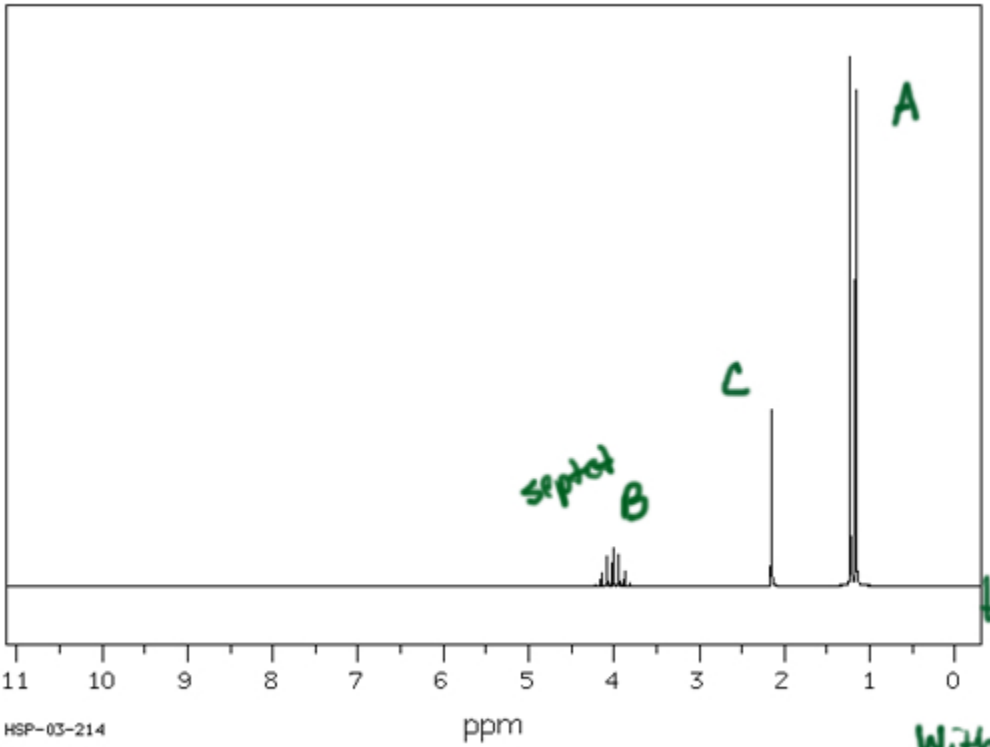
↑↓↑ ↓↑↓

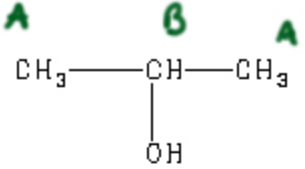
↓↑↑ ↑↓↓

+3/2 +1/2 −1/2 −3/2

n+1 rule

# of effects of n adjacent H's





C

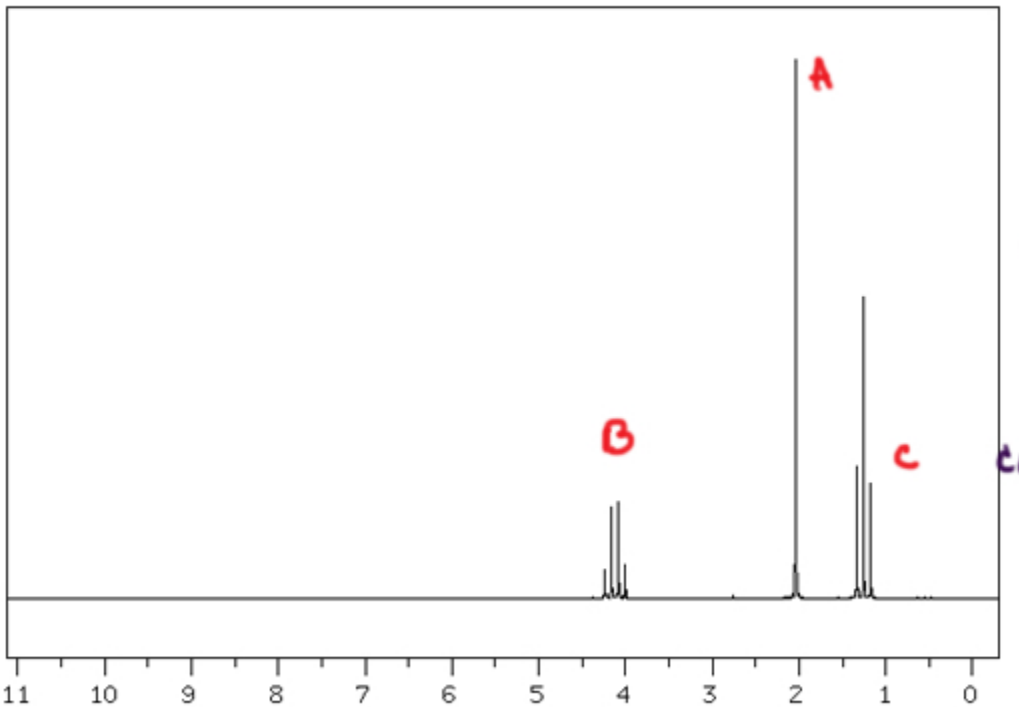
↑

acidic protons often split and they don't split others.

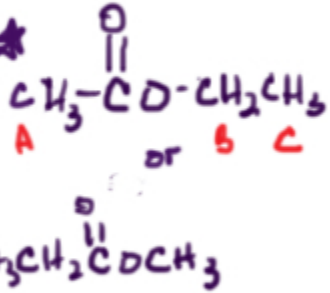
H is coming and going 100,000/s

With ^2H, C would disappear (no net spin magnetic moment)

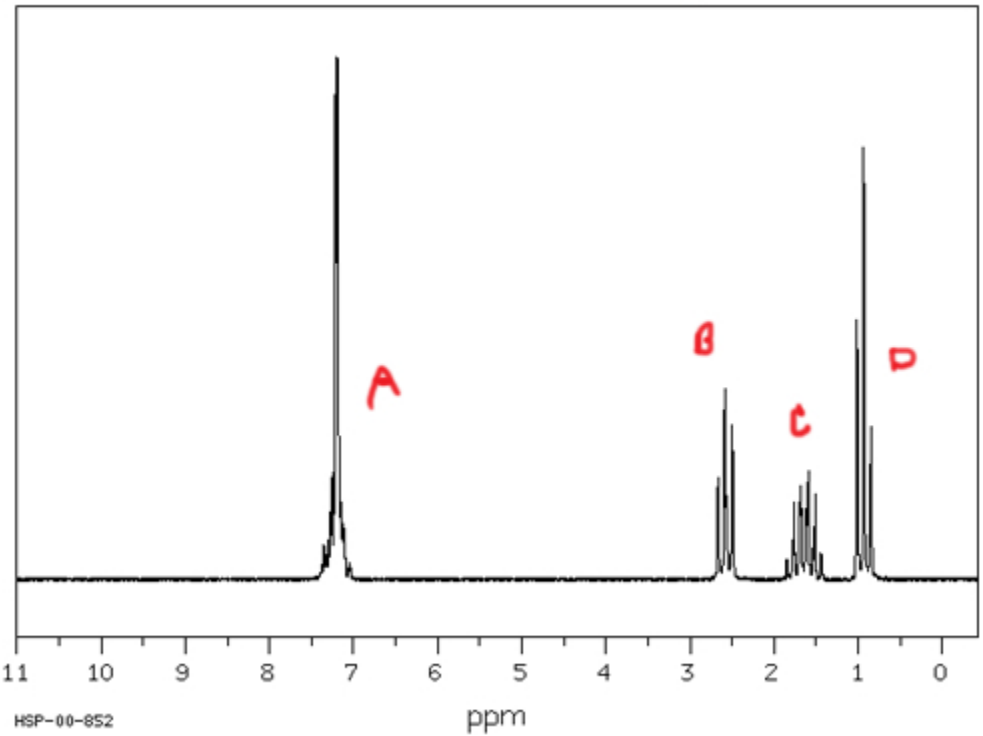
$C_4H_8O_2$

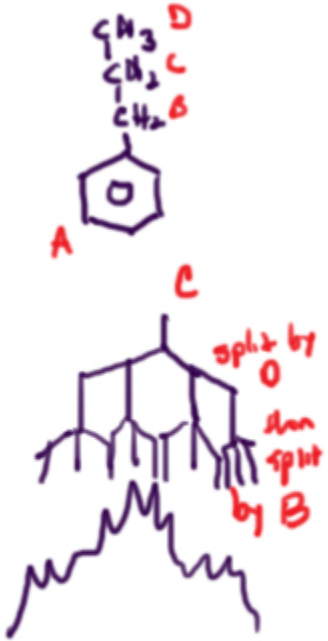


Clue: Hydrolysis yields an alcohol and an acid.

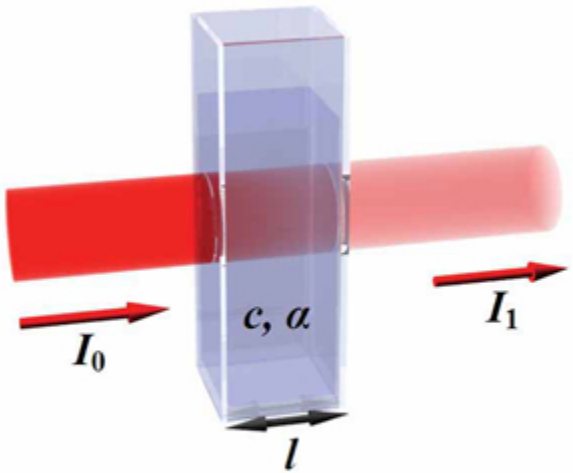


C_9H_{12}


A
B
C
D
11
10
9
8
7
6
5
4
3
2
1
0
ppm
HSP-00-852


D
C
B
A
C
split by
O
then
split
by B

UV spectroscopy



the general, microscopic description of absorption of light.

$$\log\left(\frac{I_0}{I}\right) = \epsilon c l$$

- $\frac{I_0}{I}$: what's left over
- ϵ: molar absorption
- c: concentration
- l: path length

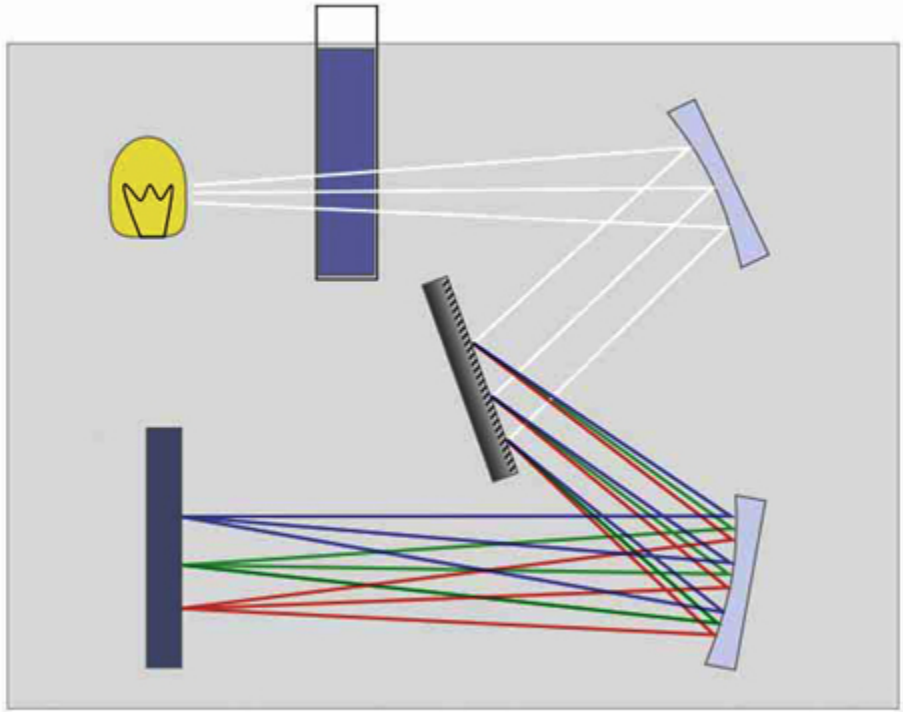
this depends on the substance and the λ of the light.

A substance will have peaks absorbance at certain λ's

This difference among substances, the peaks of absorbance, is the basis of → UV spectroscopy

$E = hf$

$f = c/\lambda$



22 JAN 2009 17:17:40 $NiCl_2(PPh_3)_2$

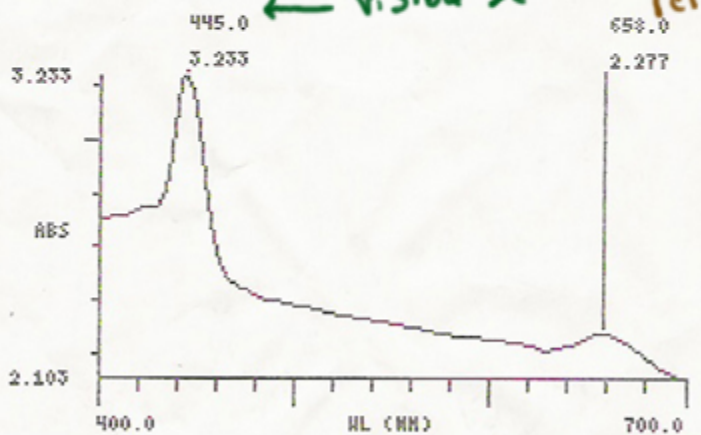
Application: SURVEY SCAN

Test name:

Data name: DEFAULT

Start Wavelength: 400.0

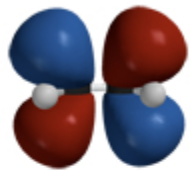
Stop Wavelength: 700.0



← visible λ

Most organic compounds, however, absorb in UV spectrum

$CH_2 = CH_2$ Ethylene



π* antibonding

LUMO

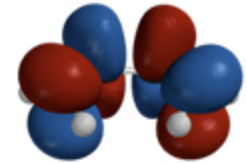
UV

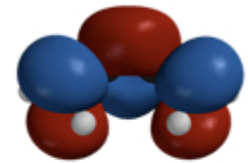
1π

HOMO

π bonding

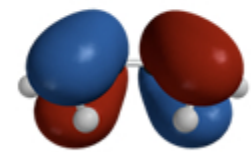
absorption peak will be broad because of thermal overtones





LUMO

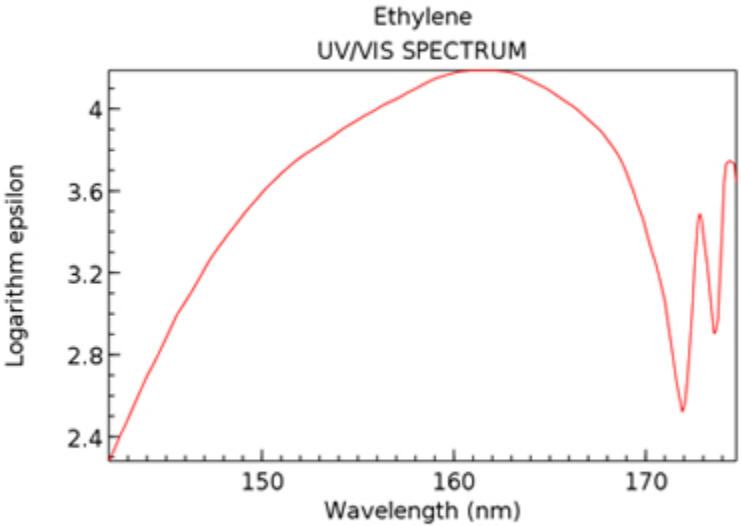
Compression of transition energy HOMO → LUMO leads to bathochromatic shift

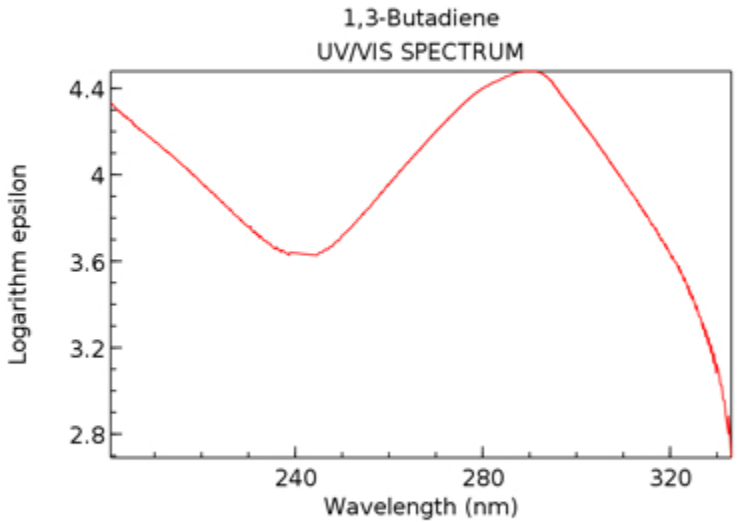


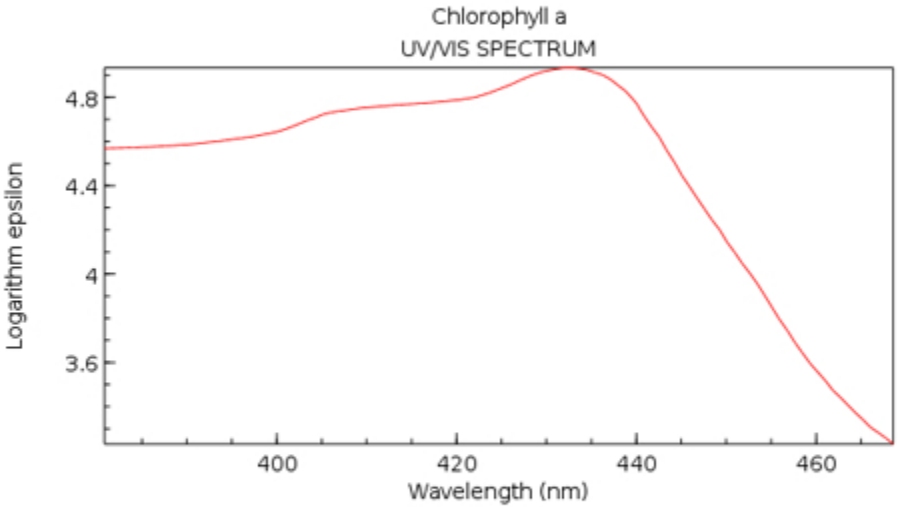
HOMO

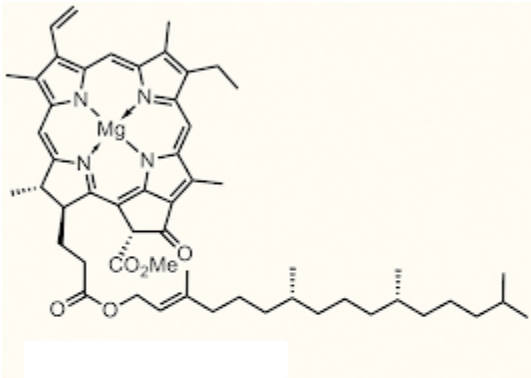
$CH_2 = CH - CH = CH_2$

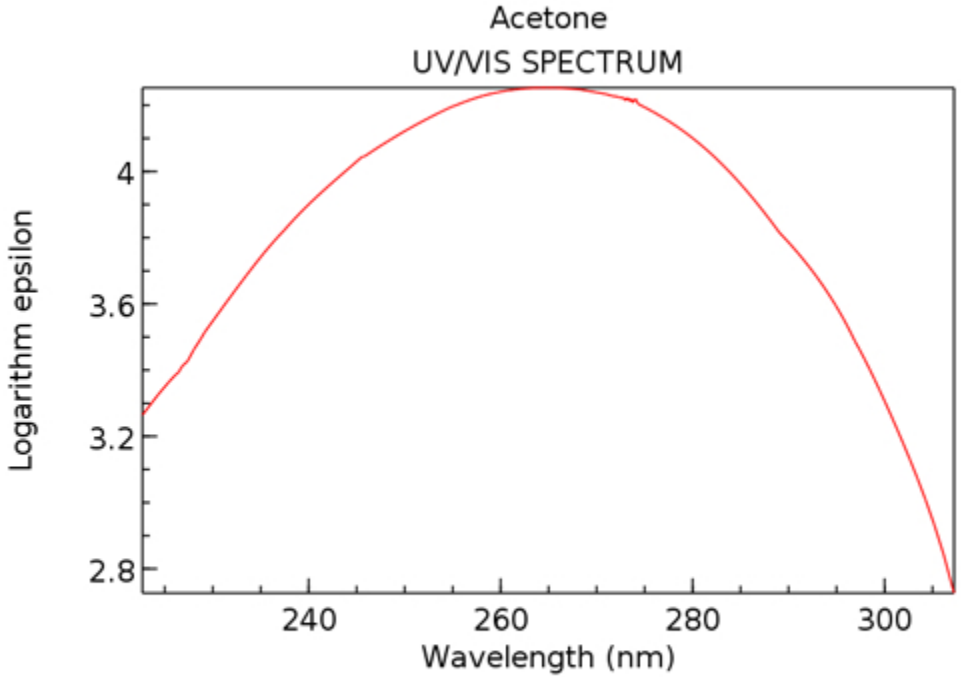
1,3 Butadiene


Ethylene
UV/VIS SPECTRUM
Logarithm epsilon
4
3.6
3.2
2.8
2.4
150
160
170
Wavelength (nm)


1,3-Butadiene
UV/VIS SPECTRUM
Logarithm epsilon
4.4
4
3.6
3.2
2.8
240
280
320
Wavelength (nm)


Chlorophyll a
UV/VIS SPECTRUM
Logarithm epsilon
4.8
4.4
4
3.6
400
420
440
460
Wavelength (nm)

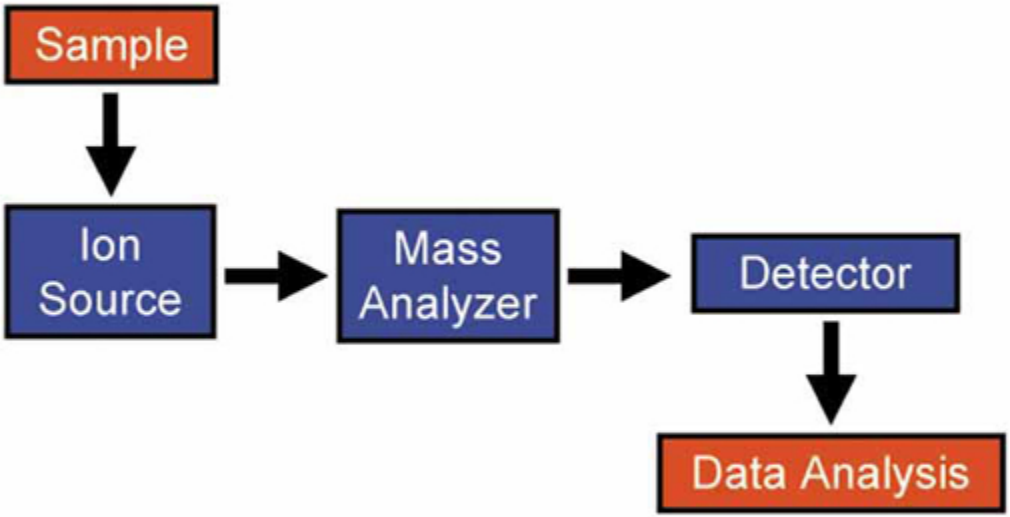

N
N
Mg
N
N
CO2Me
O
O
O



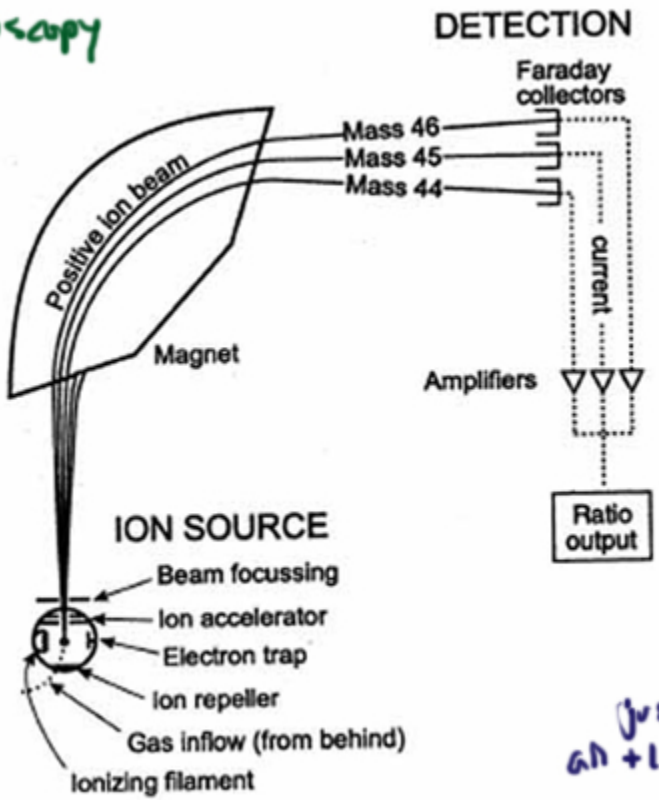
aldehydes and ketones may be brown in

π antibonding

nonbonded pair


Sample
Ion Source
Mass Analyzer
Detector
Data Analysis

Mass Spectroscopy



from sample molecule produce cations which then → fragment

Ion fragments leave ion accelerator $q = e$

$$\frac{1}{2}mv^2 = qV$$

enters magnetic field

$$F_m = qBv_\perp$$

$$F_m = F_r = \frac{mv^2}{r}$$

so, $$r = \frac{mv}{qB}$$

Combine with $\frac{1}{2}mv^2 = qV$

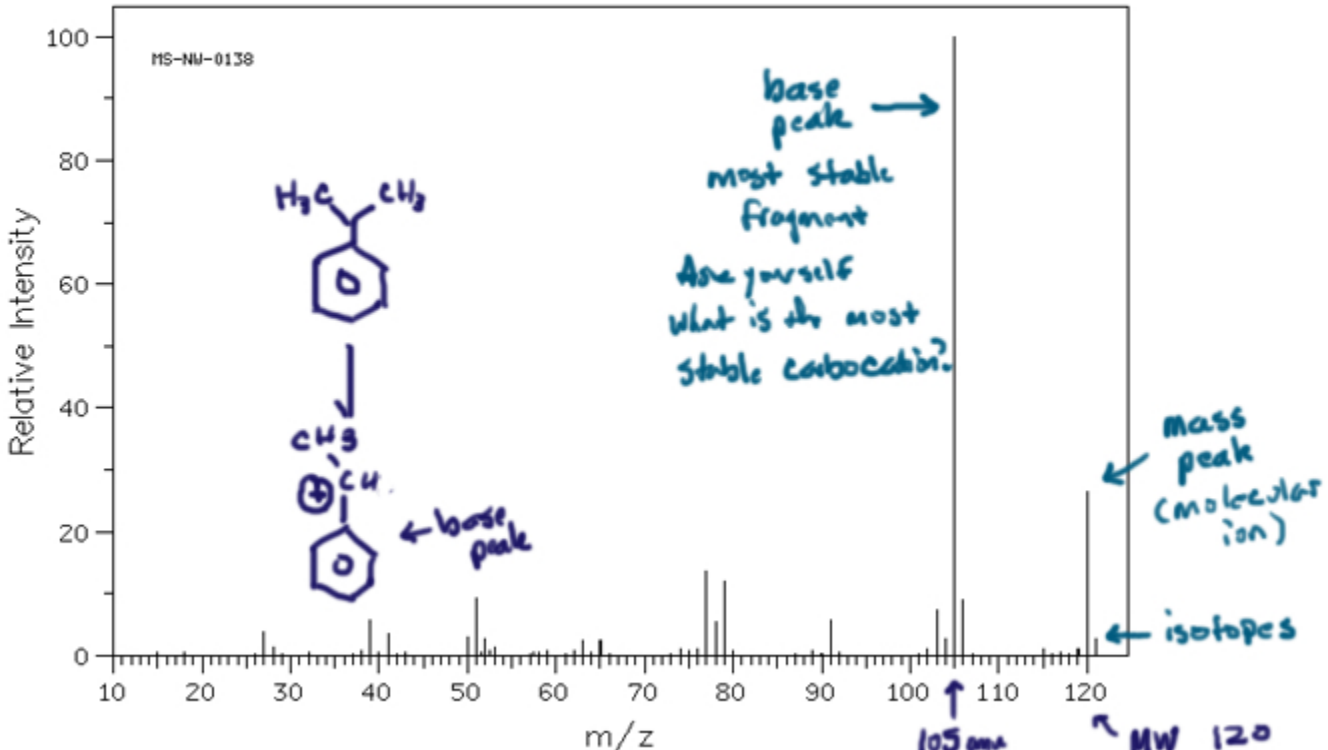
$$\frac{m}{q} = \frac{B^2r^2}{2V}$$

just e → q

all +1

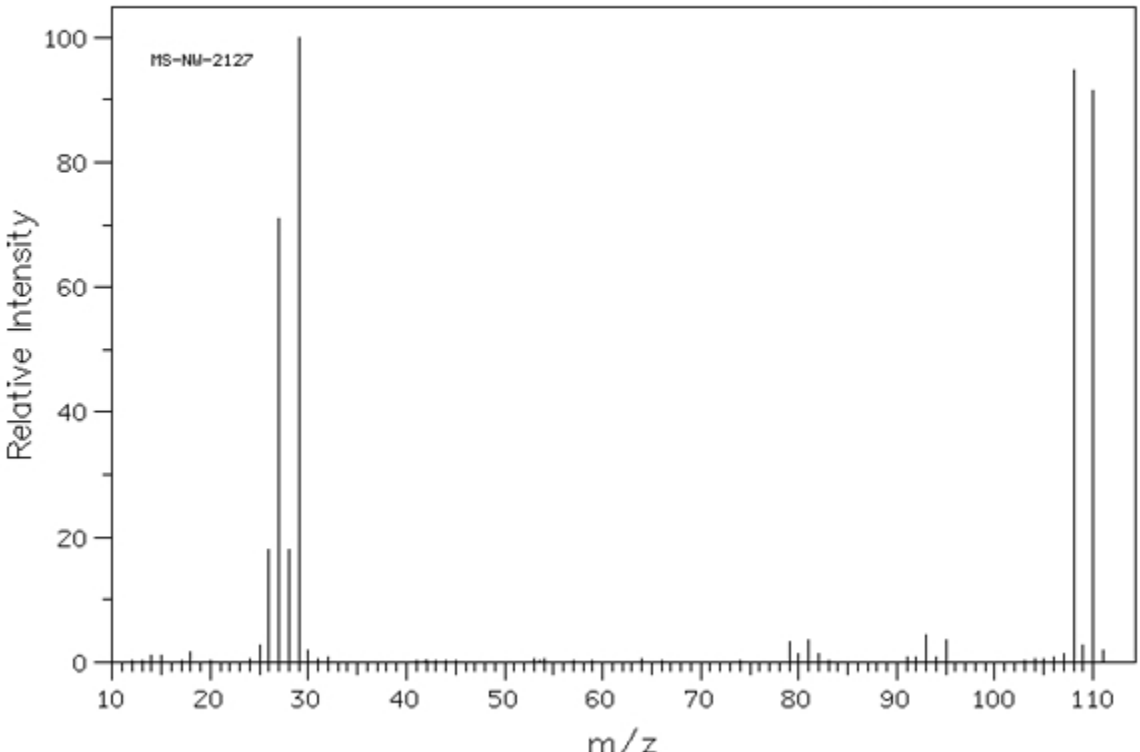
radius of curvature depends on charge to mass ratio

MS-NW-0138 SDBS NO. 1816
cumene
C9H12 (Mass of molecular ion: 120)



MS-NW-2127 SDBS NO. 901
ethyl bromide
C2H5BR (Mass of molecular ion: 108)

CH_3CH_2Br

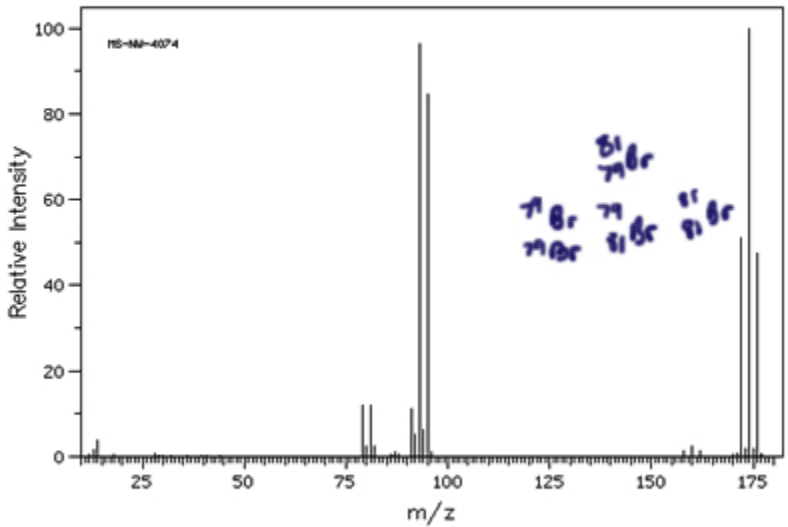


^{79}Br (50.5%)

^{81}Br (49.5%)

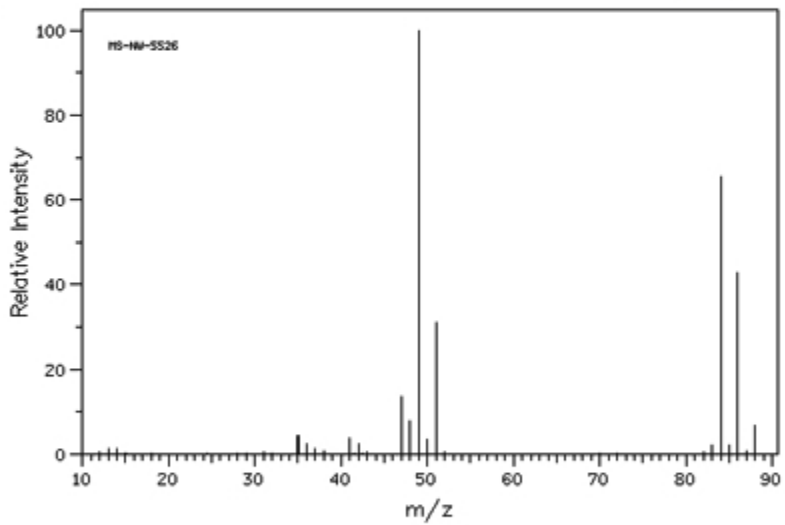
MS-NW-4074 SDBS NO. 2171
dibromomethane
CH2BR2 (Mass of molecular ion: 172)

CH_2Br_2



MS-NW-5526 SDBS NO. 891
dichloromethane
CH2CL2 (Mass of molecular ion: 84)

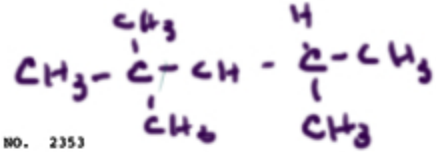
CH_2Cl_2



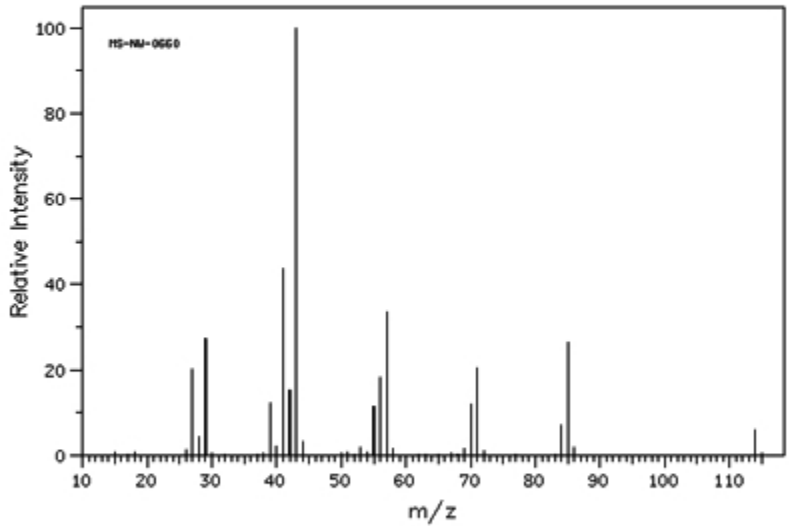
n-octane

$CH_3(CH_2)_6CH_3$

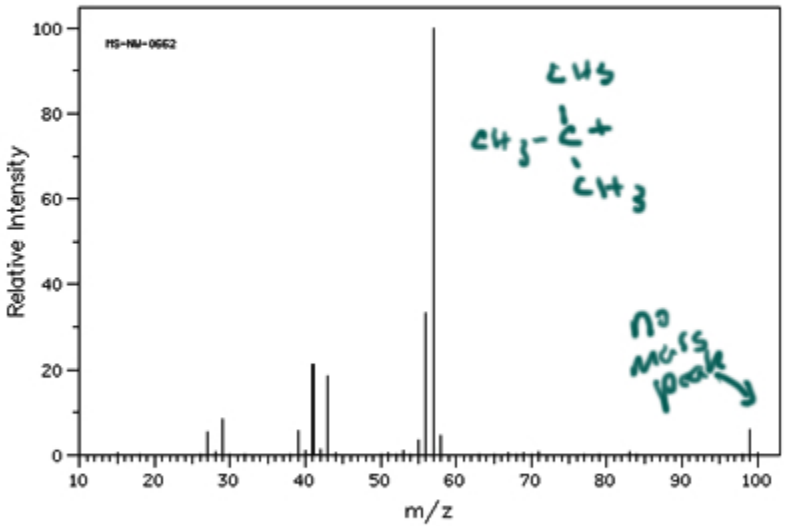
Structural isomers



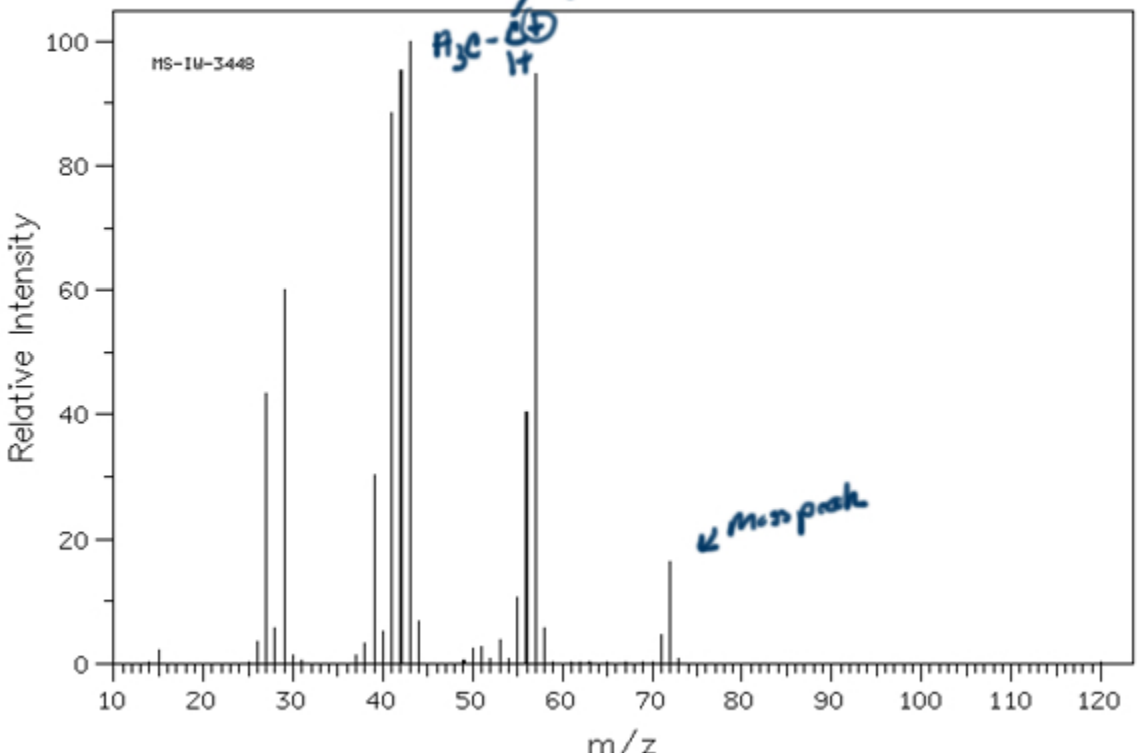
MS-NW-0660 SDBS NO. 2672
octane
C8H18 (Mass of molecular ion: 114)



MS-NW-0662 SDBS NO. 2353
2,2,4-trimethylpentane
C8H18 (Mass of molecular ion: 114)

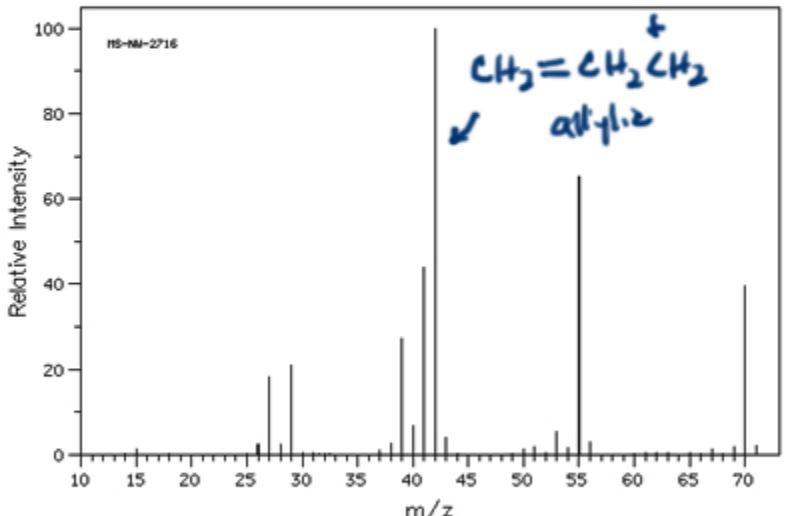


MS-IW-3448 SDBS NO. 10633
isopentane
C5H12 (Mass of molecular ion: 72)



$CH_2=CH_2CH_2\!\!\not|\!\!CH_2CH_3$

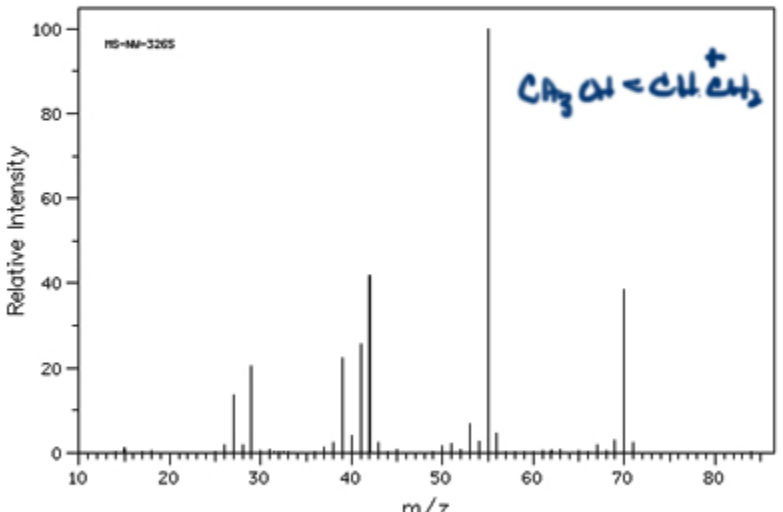
MS-NW-2716 SDBS NO. 4812
1-pentene
C5H10 (Mass of molecular ion: 70)



$CH_2=CH_2\overset{+}{C}H_2$
allyl ↙

$CH_3CH=CH\!\!\not|\!\!CH_2CH_3$

MS-NW-3265 SDBS NO. 4813
2-pentene
C5H10 (Mass of molecular ion: 70)



$CH_3CH=\overset{+}{C}HCH_3$

MS-NW-5499 SDBS NO. 1374
1-butanol
C4H10O (Mass of molecular ion: 74)

$CH_3CH_2CH_2CH_2OH$