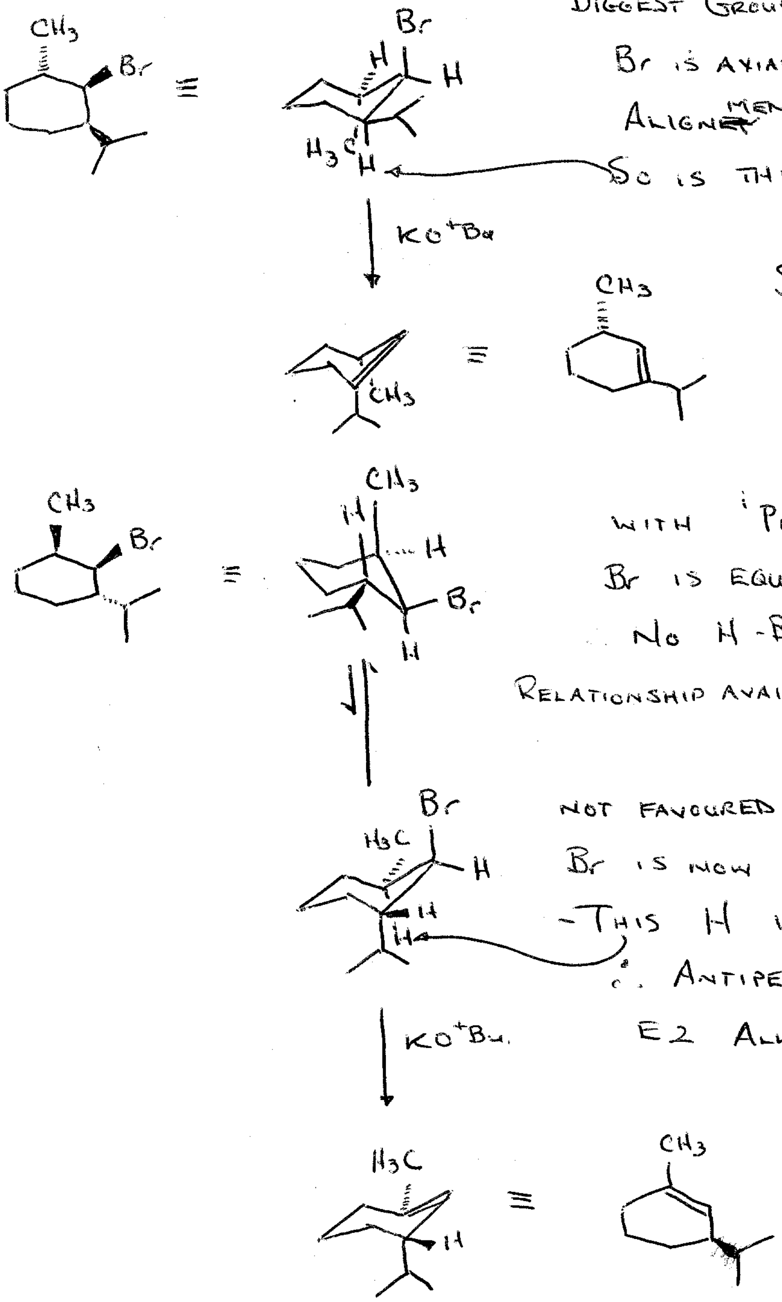
1



BIGGEST GROUP PREFERS EQUATORIAL

Br IS AXIAL - OK FOR ANTIPERIPLANAR ALIGNMENT FOR E2

SO IS THIS H ATOM (ONLY)

SHOULD BE RELATIVELY FAST

WITH ^{i}Pr GROUP EQUATORIAL

Br IS EQUATORIAL TOO

NO H-Br ANTIPERIPLANAR RELATIONSHIP AVAILABLE WITHOUT A 'RING FLIP'

NOT FAVOURED CONFORMATION, BUT

Br IS NOW AXIAL

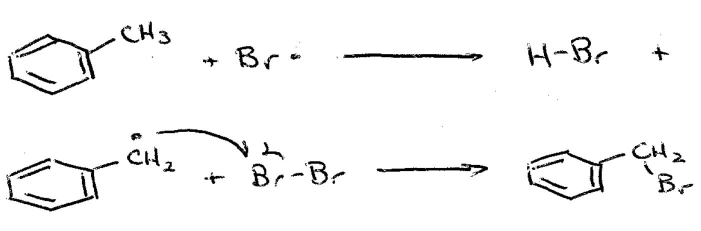
- THIS H IS NOW AXIAL, TOO

∴ ANTIPERIPLANAR H AND Br

E2 ALLOWED

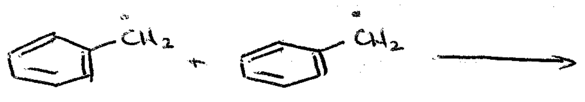
BUT MUST BE CONSIDERABLY SLOWER.

2. $Br_2 \xrightarrow{h\nu} 2\,Br\cdot$ INITIATION



PROPAGATION

NOTE: BENZYL RADICAL RESONANCE FORMS NOT NECESSARY, BUT MUST BE CORRECT IF DRAWN

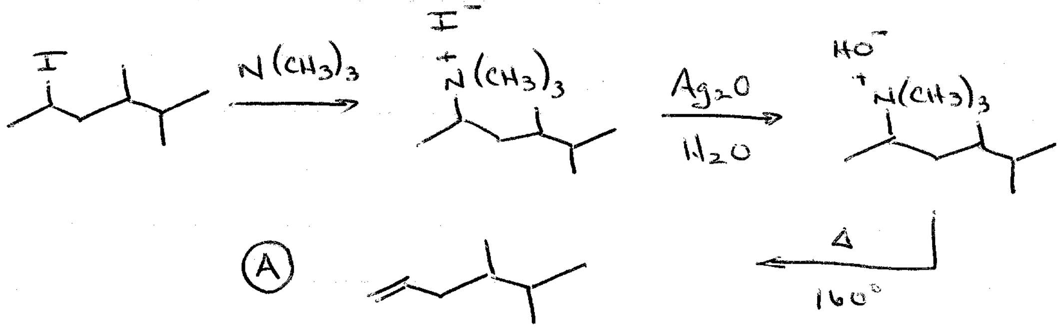


TERMINATION

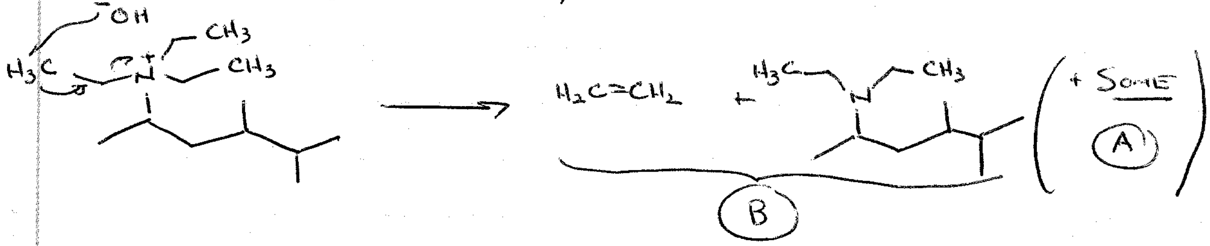
IS ALSO ACCEPTABLE

$Br\cdot + Br\cdot \longrightarrow Br_2$ WILL ALSO DO, ALTHOUGH I DON'T MUCH LIKE IT.

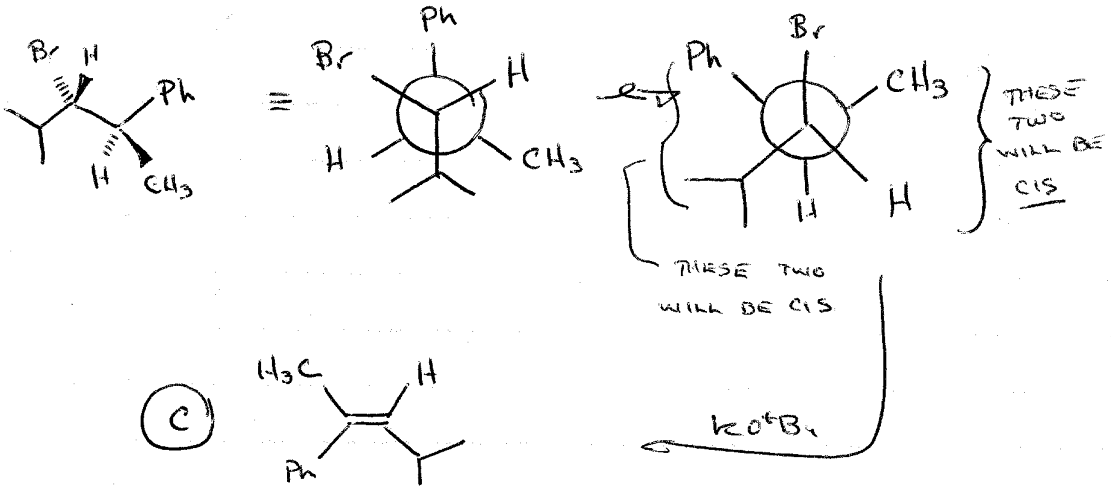
3 a)



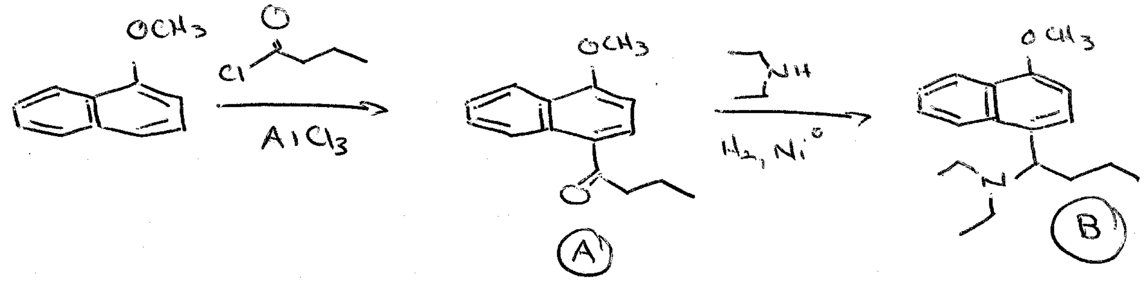
IF $N(CH_2CH_3)_3$ WAS USED, YOU'D HAVE COMPETITION FROM,



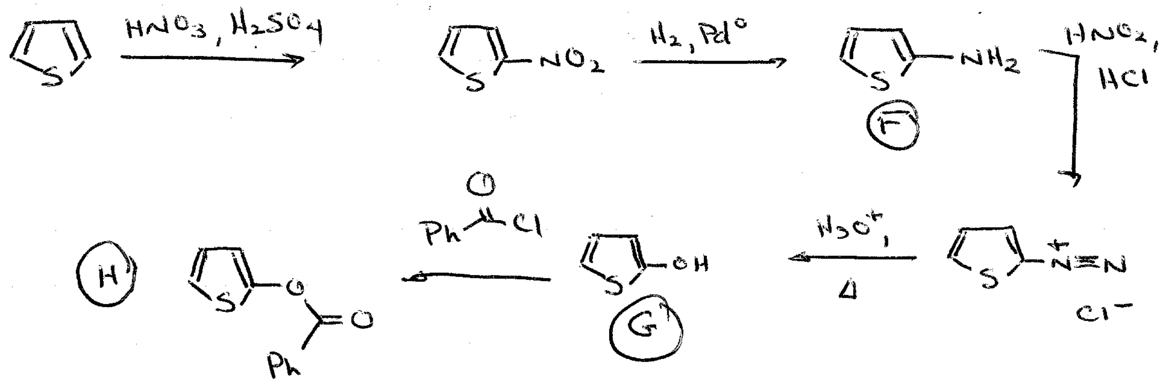
b)



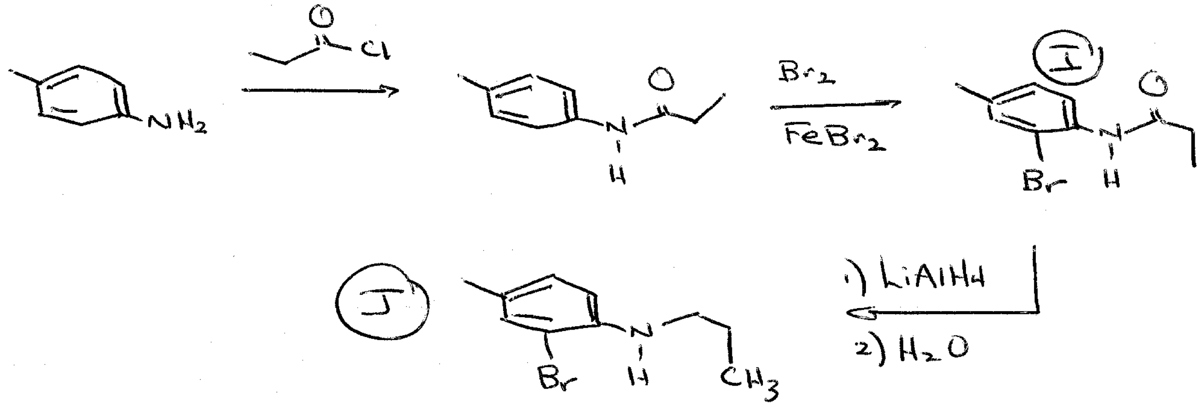
c)


OCH3
Cl
O
AlCl3
OCH3
O
A
NH
H2, Ni°
OCH3
N
B

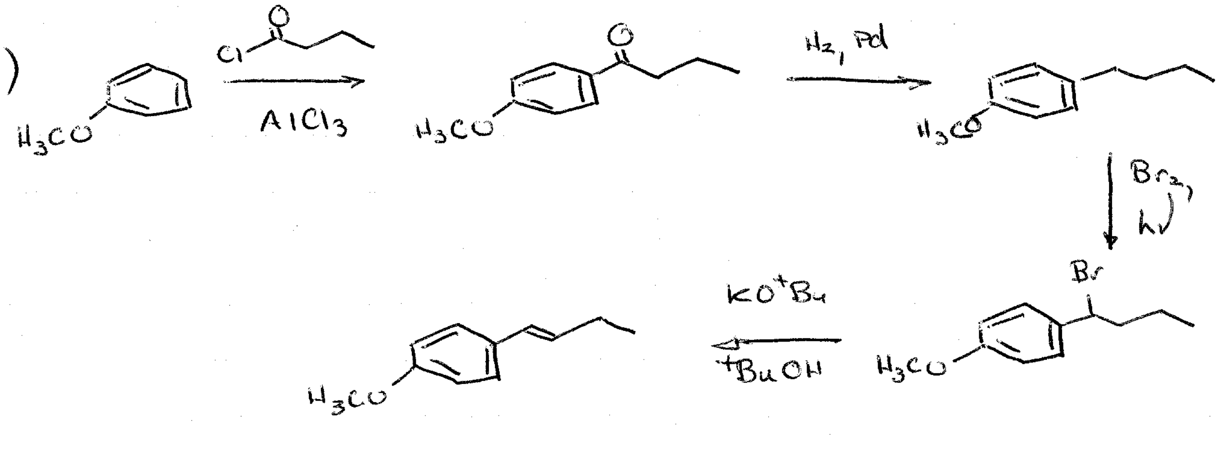
d)


S
HNO3, H2SO4
S
NO2
H2, Pd°
S
NH2
F
HNO2, HCl
S
N≡N +
Cl−
H3O+, Δ
S
OH
G
Ph
O
Cl
H
S
O
O
Ph

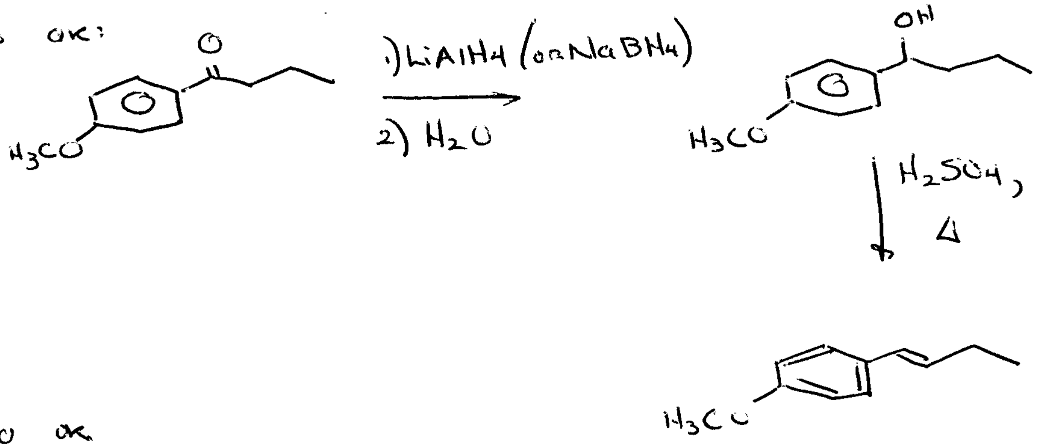
e)


NH2
O
Cl
N
H
O
Br2
FeBr2
I
N
O
Br
H
1) LiAlH4
2) H2O
J
N
Br
H
CH3

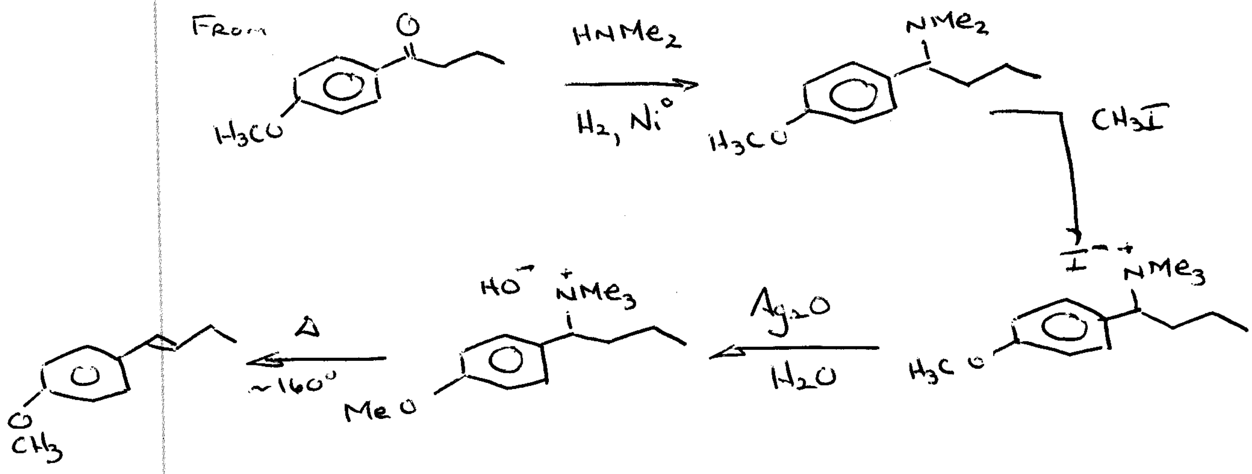
4 a)


H3CO
Cl
O
AlCl3
O
H3CO
H2, Pd
H3CO
Br2, hν
Br
H3CO
KOtBu
tBuOH
H3CO

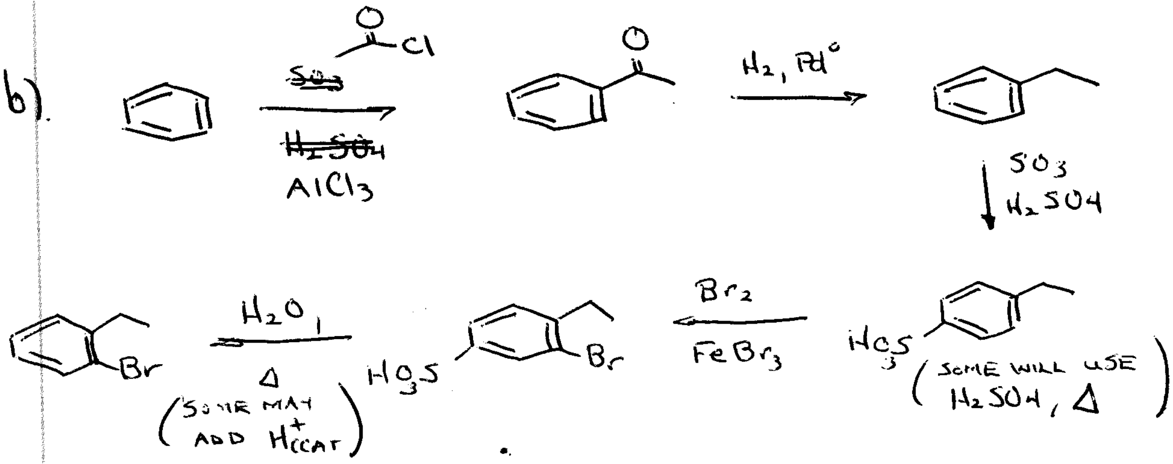
ALSO OK:
FROM



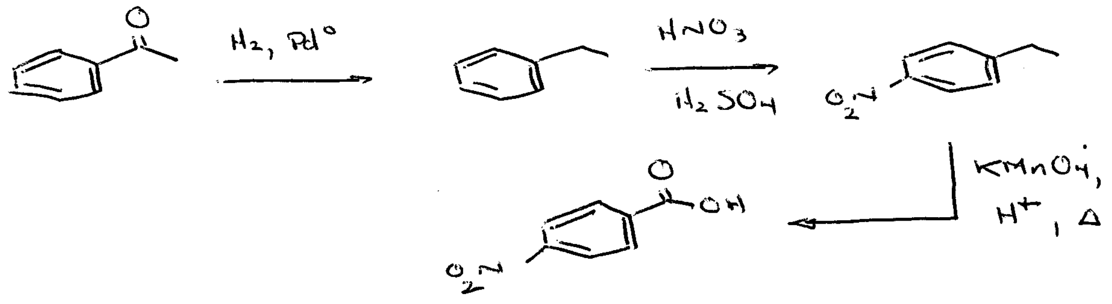
ALSO OK
FROM



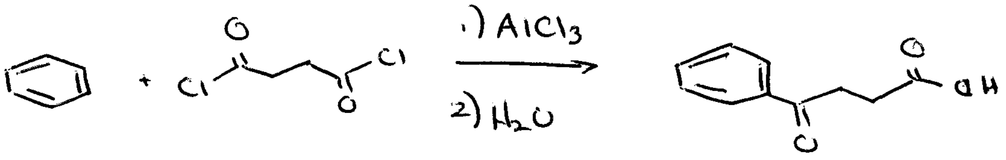
b).



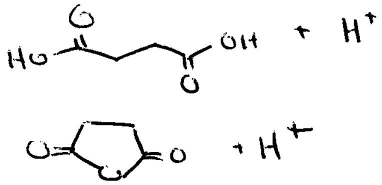
c)

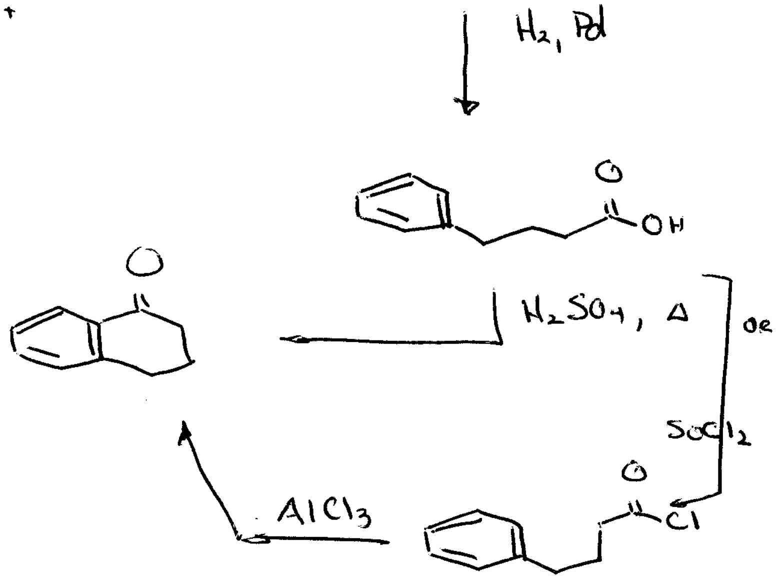


d)

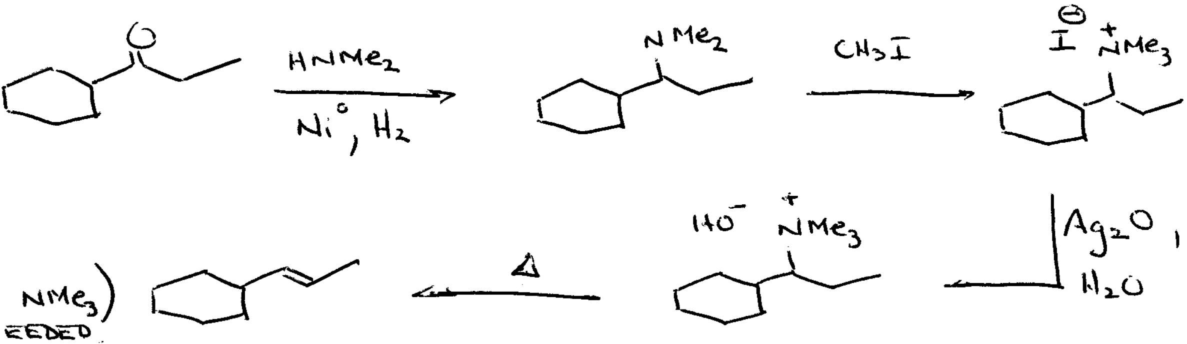


NOTE: MAY USE



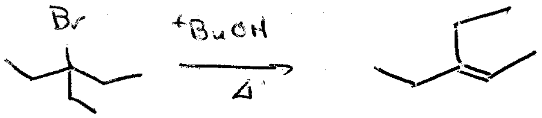


e)



($+H_2O + NMe_3$)
NOT NEEDED

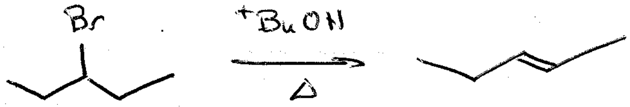
5



3° ALKYL HALIDE - CARBOCATION 'STABILIZING'

BASE IS VERY POOR - ESSENTIALLY A NON-BASE

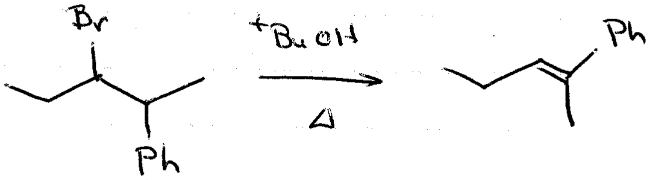
∴ VERY HIGH E1 CHARACTER



2° ALKYL HALIDE - 2° CARBOCATION WOULD BE LESS STABLE

BASE IS STILL LOUSY

∴ STILL HIGH DEGREE OF E1, BUT LESS THAN ABOVE CASE

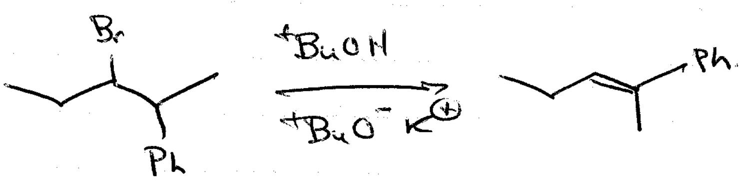


2° ALKYL HALIDE - 2° CARBOCATION MUCH LIKE ABOVE

<u>BUT</u> Ph GROUP AT β- POSITION ACIDIFIES β-H

∴ A BIT MORE PRONE TO E2

∴ 2ND MOST E2 CHARACTER



BASE NOW AN EXCELLENT ONE - THE PROTOTYPICAL E2 BASE

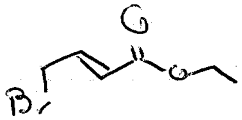
Ph AT β- POSITION ALSO ENCOURAGES E2 ∴ GOES INTO CONJUGATION

∴ MOST E2

6. FROM ELEMENTAL ANALYSIS:

	C	H	Br	O
	36.95	5.68	40.97	16.40
÷	12.011	÷ 1.008	÷ 79.904	÷ 15.999
=	3.076	= 5.6349	= 0.512	= 1.025
÷ BY SMALLEST	÷ 0.512	÷ 0.512	÷ 0.512	÷ 0.512
	6.01	11.00	1	2.00

∴ EMPERICAL FORMULA IS $C_6 H_{11} Br_1 O_2$

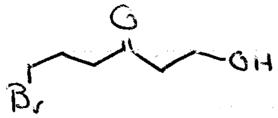
∴ CAN ELIMINATE  $C_6H_9BrO_2$

OTHERS FIT

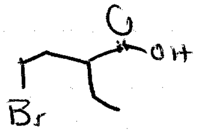
NOW TO IR:

MOST IMPORTANT BAND IS.

ν_{MAX} 1740 cm^{-1} - ALMOST CERTAINLY C=O STRETCH OF ESTER.

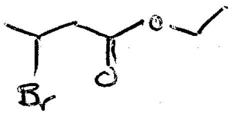
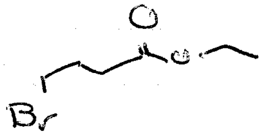
∴  IS OUT $\nu_{C=O}$ 1710 cm^{-1} PREDICT

ν_{OH} (~3400 cm^{-1}) ALSO MISSING.

 IS ALSO OUT $\nu_{C=O}$ ~1700 cm^{-1}

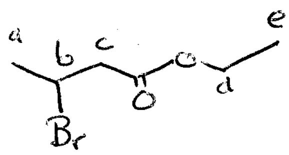
ν_{OH} (3000 cm^{-1}) ALSO MISSING.

MIGHT AS WELL ASSIGN THE ν_{MAX} = 2978 cm^{-1} BAND HERE IT'S C-H STRETCH OF THE ALIPHATIC sp^3C-H 'S.

∴  AND 

STILL ELIGIBLE.

TO ¹H NMR.

LET'S TRY 

FIRST

FOR H_a PREDICT δ = $\underset{(CH_3)}{0.8} + \underset{(M\text{-}C\text{-}Br)}{1.0}$ = 1.8 ppm, DOUBLET, A = 3

NO DOUBLETS ANYWHERE — PROBLEM

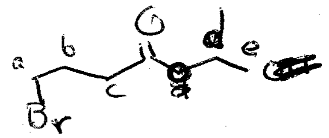
TRY ONE MORE

H_b PREDICT δ = $\underset{(CH)}{1.6} + \underset{(M\text{-}Br)}{2.5} + \underset{(M\text{-}C\text{-}CO_2R)}{0.3}$ = 4.4 ppm,

TRIPLET OF QUARTETS, A = 1

- ONLY THING NEAR 4.4 ppm IS AN A = 2 QUARTET

— DOES NOT FIT.

TRY 

FOR H_a, PREDICT δ = $\underset{(CH_2)}{1.2} + \underset{(M\text{-}Br)}{2.2}$ = 3.4 ppm, TRIPLET, A = 2

GOOD AGREEMENT WITH δ 3.45, d, A = 2 PEAK PRESENT

H_b, PREDICT δ = $\underset{(CH_2)}{1.2} + \underset{(M\text{-}C\text{-}Br)}{0.7} + \underset{(M\text{-}C\text{-}CO_2R)}{0.5}$ = 2.4 ppm,

TRIPLET OF TRIPLETS, A = 2

OK AGREEMENT WITH δ2.17 (m, A = 2) PEAK PRESENT

H_c, PREDICT δ = $\underset{(CH_2)}{1.2} + \underset{(M\text{-}CO_2R)}{1.0}$ = 2.2 ppm, TRIPLET, A = 2

ACCEPTABLE AGREEMENT WITH δ2.50 (t, A = 2) PEAK PRESENT

Hd, PREDICT $\delta = \underset{(CH_2)}{1.2} + \underset{(M-O-\underset{\overset{\|}{O}}{C}-R)}{2.9} = 4.1$ ppm, QUARTET, A=2

GOOD AGREEMENT WITH δ 4.15 (q, A=2) PEAK PRESENT

He, PREDICT $\delta = \underset{(CH_3)}{0.8} + \underset{(M-C-O\underset{\overset{\|}{O}}{C}R)}{0.5} = 1.3$ ppm, QUARTET, A=3.

GOOD AGREEMENT WITH δ 1.26 (t, A = 3) PEAK PRESENT

ALL ABSORPTIONS HAVE AT LEAST ACCEPTABLE AGREEMENT WITH ^{1}H SPECTRUM PRESENTED

∴ COMPOUND IS