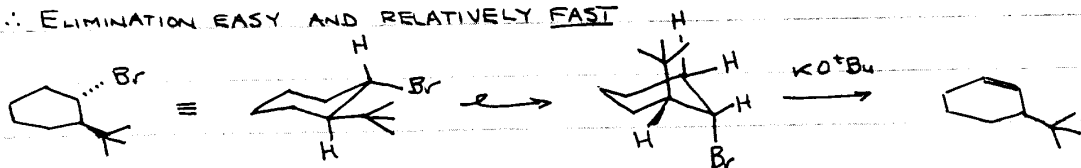


^tBUTYL GROUP EQUATORIAL ~~X~~ ALLOWS Br TO BE AXIAL ∴ CAN GET TO AN ANTIPERIPHERAL ORIENTATION WITH RESPECT TO H ATOM ON NEXT CARBON

∴ ELIMINATION EASY AND RELATIVELY FAST

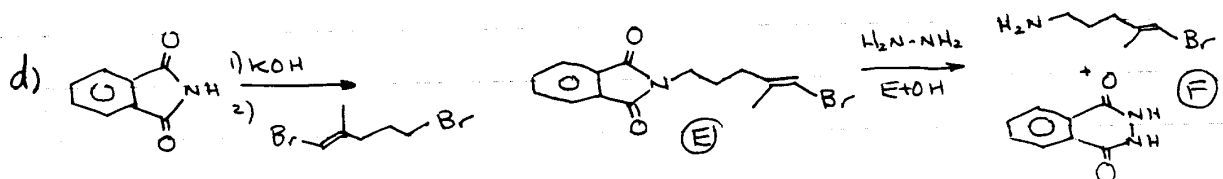
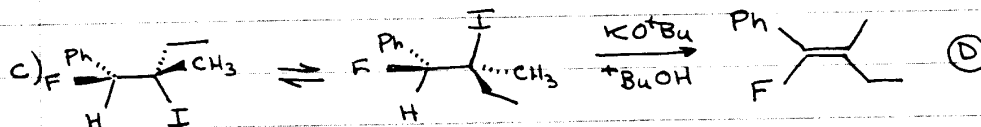
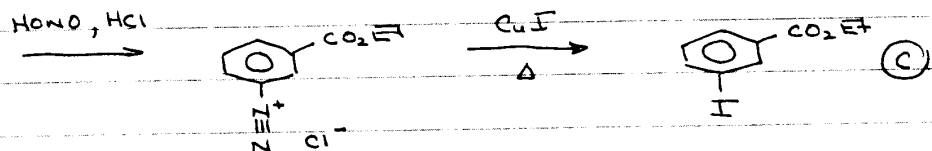
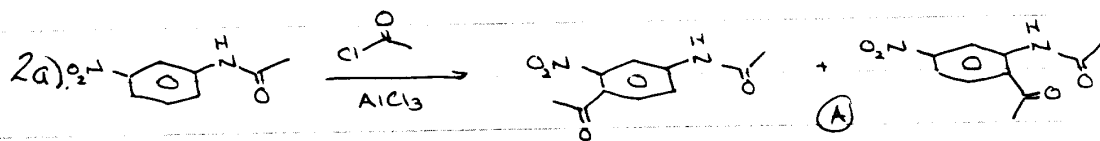


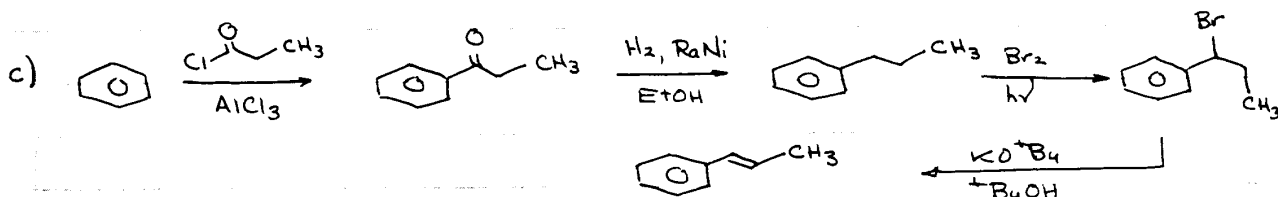
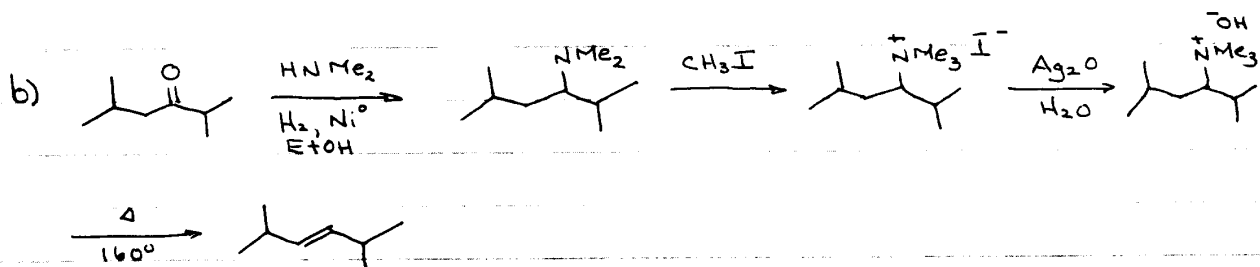
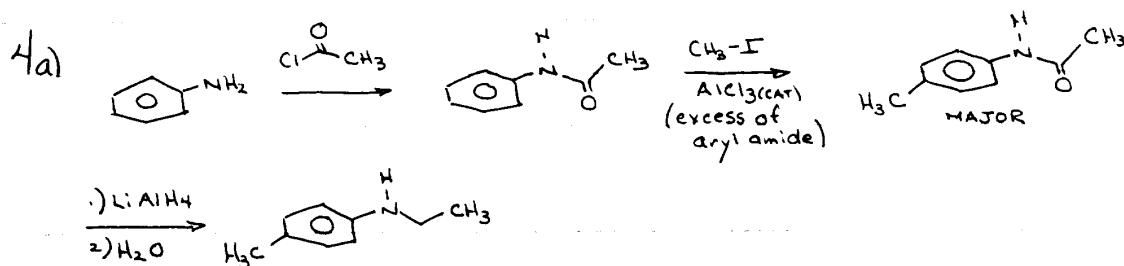
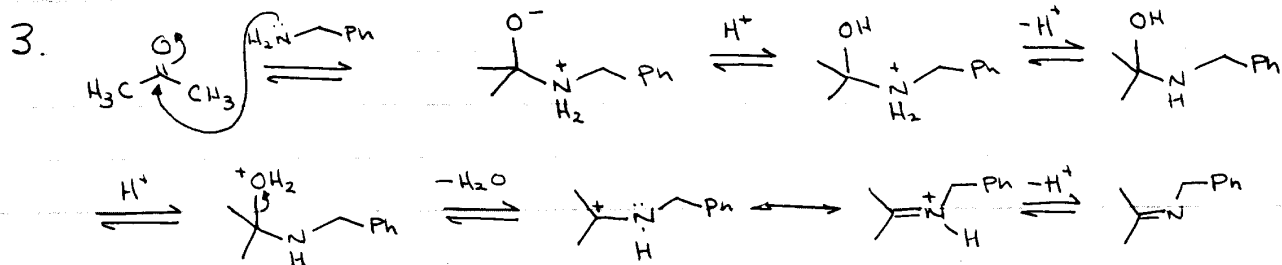
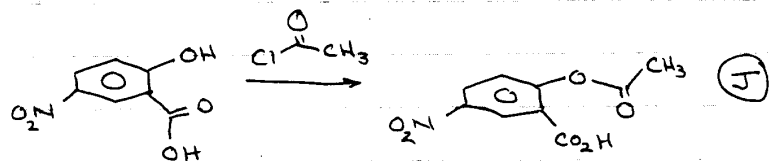
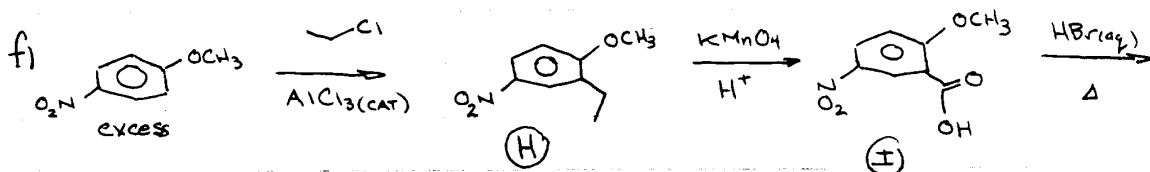
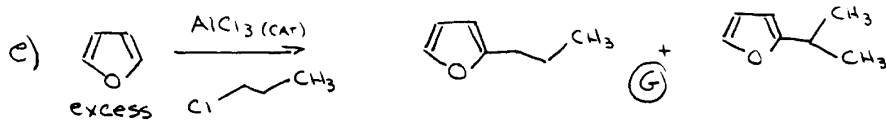
IN GROUND STATE CONFORMATION (^tBUTYL EQUATORIAL), Br IS EQUATORIAL

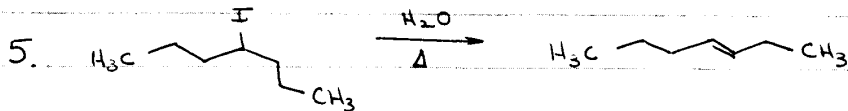
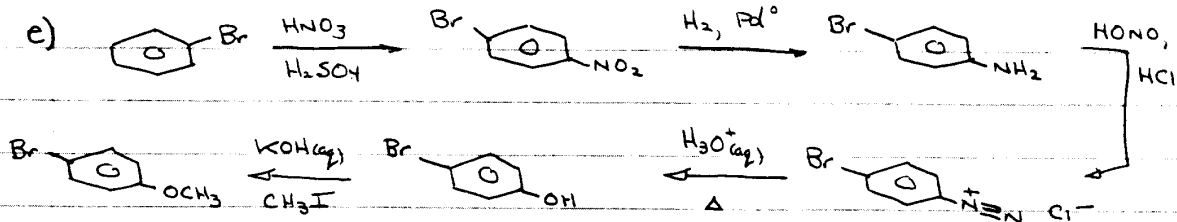
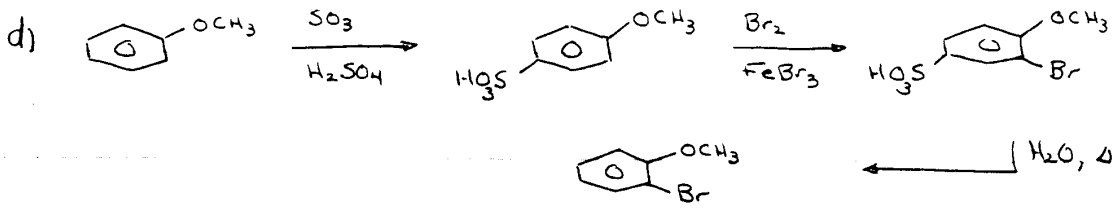
- RING MUST FLIP TO GET AXIAL Br AND ANTIPERIPHERAL H, Br ORIENTATION.

THIS IS TOUGH, SINCE IT FORCES ^tBUTYL AXIAL ∴ ELIMINATION SLOW

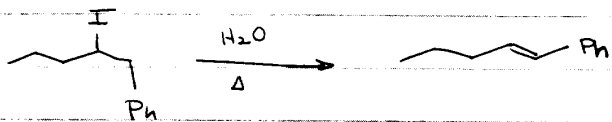
STRONG BASE, Br LEAVING GROUP ⇒ E2 ELIMINATION



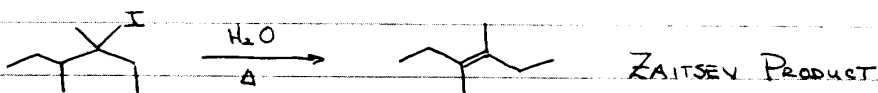




- INTERMEDIATE CASE: 2° ALKYL HALIDE, 1 SUBSTITUENT AT β POSITION



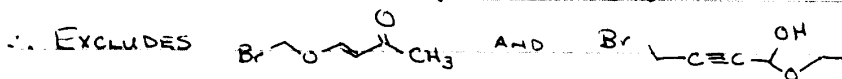
- 2° ALKYL HALIDE; β -POSITION HAS ARYL GROUP, WHICH SPEEDS UP E2
 \therefore MOST E2 CHARACTER



- 3° ALKYL HALIDE \therefore CATION STABILIZATION - FAVOURS E1 MOST

6. IR ANALYSIS \checkmark MAX OF CARBONYL AT 1714 cm^{-1}

\therefore COMPOUND MUST CONTAIN NON-CONJUGATED KETONE ($\nu_{\text{MAX}} \approx 1710$) OR ACID OR A CONJUGATED ESTER ($1735 - 1755 \text{ cm}^{-1}$)



ALSO EXCLUDES BrCC(=O)C#C SINCE THERE'S NO $\nu_{\text{C}\equiv\text{C}}$ ($\sim 2200 \text{ cm}^{-1}$)

ANALYSIS DATA.

C 37.33	H 4.70	Br 41.39	O 16.58
$\div 12.011$	$\div 1.008$	$\div 79.904$	$\div 15.999$
= 3.11	= 4.66	= 0.518	= 1.04

\div SMALLEST VALUE

$\div 0.518$	$\div 0.518$	$\div 0.518$	$\div 0.518$
= 6.01	= 9.00	= 1	= 2.01

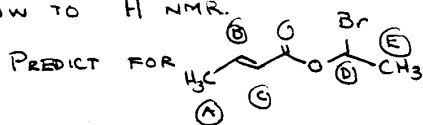
\therefore EMPIRICAL FORMULA IS $C_6H_9BrO_2$

NOTE: COULD CONCEIVABLY BE $C_{12}H_{18}Br_2O_4$

THIS EXCLUDES. BrC=C(C)C(=O)OCH3 $C_6H_7BrO_2$

\therefore LEAVES BrC=C(C)C(=O)OCH2CH3 AND BrC=CC(=O)OCH2CH3 POSSIBLE

NOW TO 1H NMR.



(A) $\delta = 1.6$ ppm (DOUBLET, AREA = 3)

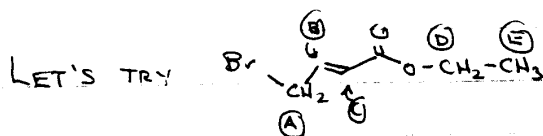
(B) $\delta = 6.9$ ppm (DOUBLET OF QUARTETS, AREA = 1)

(C) $\delta = 6.0$ ppm (DOUBLET, AREA = 1)

(D) $\delta = 4.5 + 2.5 = 7.0$ ppm (QUARTET, AREA = 1)

(E) $\delta = 1.3 + 1.0 = 2.3$ ppm (DOUBLET, AREA = 3)

DOESN'T FIT AT ALL OBSERVED SPECTRUM, ESPECIALLY OBSERVED PEAKS AT δ 1.3 (TRIPLET, AREA = 3), 4.0 (DOUBLET, AREA = 2) AND 4.2 (QUARTET, AREA = 2)

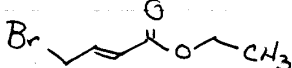


PREDICT

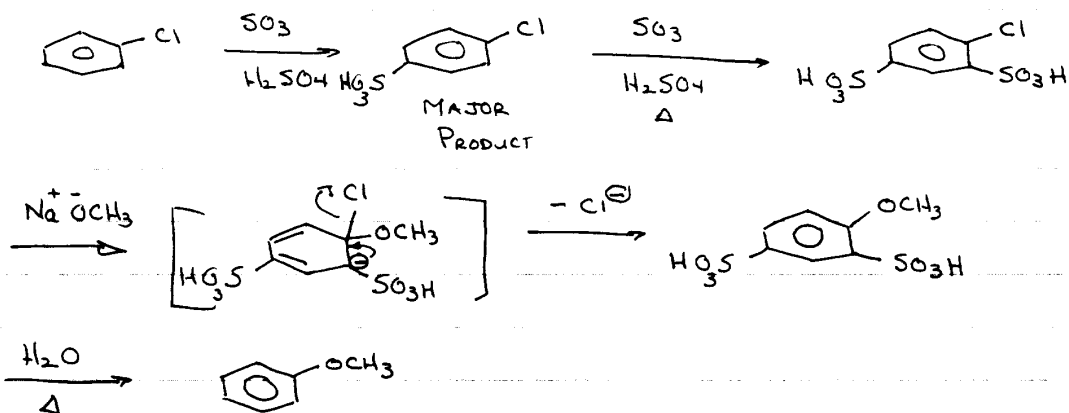
(A) $\delta = 2.0 + 2.2 = 4.2$ ppm (DOUBLET, AREA = 2)

- REASONABLE AGREEMENT WITH δ 4.0 ppm DOUBLET

- (B) $\delta = 6.9 \text{ ppm}$ (DOUBLET OF TRIPLETS, AREA = 1)
 - EXCELLENT AGREEMENT WITH $\delta = 7.0 \text{ ppm}$ RESONANCE (5 LINE ABSORBANCE).
- (C) $\delta = 6.0 \text{ ppm}$ (DOUBLET, AREA = 1)
 - EXCELLENT AGREEMENT WITH $\delta = 6.0 \text{ ppm}$ DOUBLET
- (D) $\delta = (\text{CH}_2 - \overset{\text{O}}{\parallel} \text{C} - \text{R}) = 4.2 \text{ ppm}$ (QUARTET, AREA = 2)
 - EXCELLENT AGREEMENT WITH $\delta = 4.2 \text{ ppm}$ QUARTET
- (E) $\delta (\text{CH}_3 - \overset{\text{O}}{\parallel} \text{C} - \text{R}) = 1.3 \text{ ppm}$ (TRIPLET, AREA = 3)
 - EXCELLENT AGREEMENT WITH $\delta = 1.3 \text{ ppm}$ TRIPLET

\therefore COMPOUND IS CLEARLY 

BONUS: YOU'D LIKE TO DO NUCLEOPHILIC AROMATIC SUBSTITUTION. SINCE BENZENE RINGS ARE ELECTRON RICH, THIS DOESN'T OCCUR EASILY, UNLESS YOU PUT AT LEAST ONE (AND PREFERABLY MORE) ELECTRON WITHDRAWING GROUPS ON THE RING. SO....



NOTE: NITRO (NO_2) GROUPS CAN ALSO SERVE THIS PURPOSE