

UNIVERSITY OF CALGARY  
FACULTY OF SCIENCE  
FINAL EXAMINATION  
CHEMISTRY 353

Version

1

April 26th, 2019

Time: 3 Hours

READ THE INSTRUCTIONS CAREFULLY

PLEASE WRITE YOUR NAME & STUDENT I.D. NUMBER ON **BOTH** YOUR BLUE ANSWER BOOKLET AND COMPUTER ANSWER SHEET.

ENTER VERSION NUMBER 1 ON THE COMPUTER ANSWER SHEET

The examination consists of Parts **1 - 10**, each of which should be attempted. Note that some Parts provide you with a choice of questions, e.g. answer 5 out of 6. These will be graded in order the answers appear until the required number have been completed, **regardless** of whether they are right or wrong.

Parts **1 - 6** will be computer graded, and Parts **7 - 10** are to be answered in the blue answer booklet. Parts **1 - 6** consist of a series of multiple choice questions numbered **1 - 49** which are to be answered on your optical score answer sheet. Indicate your answer by blackening out the appropriate space, A, B, C, D or E on the answer sheet. Use a pencil only and **not ink**. In some cases it is required that you indicate **multiple** items for a complete and/or correct answer by blackening out more than one space. In some other cases more than five options are available and some of these also require more than one space to be blackened out. For an example, an option specified as AB requires that you blacken out **both** space A and space B. Part marks may be awarded in some of the questions. Incorrect answers must be erased **cleanly**.

A periodic table with atomic numbers and atomic weights and tables of spectroscopic data are provided at the end of the examination paper. **No other resources are allowed.**

Molecular models and calculators are permitted, **but NOT programmable calculators**. **Absolutely no other electronic devices are allowed.**

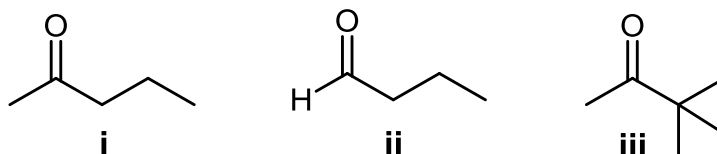
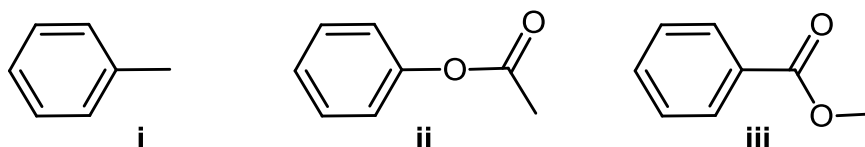
12% **PART 1: RELATIVE PROPERTIES**

ANSWER ANY EIGHT (8) OF THE TEN (10) QUESTIONS 1-10.

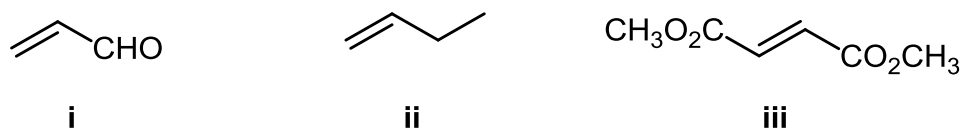
Arrange the items in questions 1-10 in **DECREASING ORDER** (*i.e.* greatest, most *etc.* *first*) with respect to the indicated property. Use the following code to indicate your answers in the box provided:

<b>A</b>	<b>i &gt; ii &gt; iii</b>	<b>D</b>	<b>ii &gt; iii &gt; i</b>
<b>B</b>	<b>i &gt; iii &gt; ii</b>	<b>E</b>	<b>iii &gt; i &gt; ii</b>
<b>C</b>	<b>ii &gt; i &gt; iii</b>	<b>AB</b>	<b>iii &gt; ii &gt; i</b>

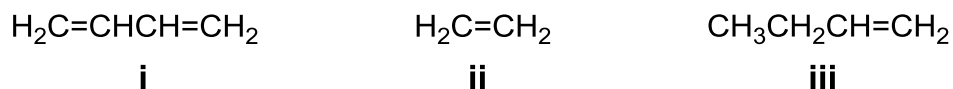
1. The relative reactivity of each of following towards sodium borohydride:

2. The relative rate of reaction of  $(\text{CH}_3)_3\text{CCl} / \text{AlCl}_3$  with each of the following:

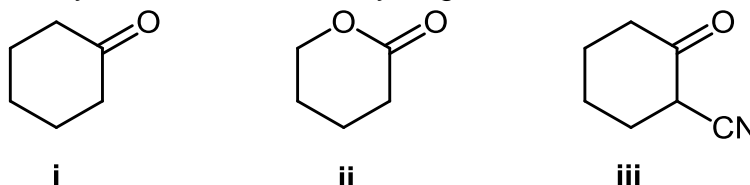
3. The relative reactivity of each of the following towards 1,3-butadiene:



4. The relative reactivity of each of the following towards HCl:



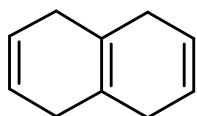
5. The relative acidity of the most acidic hydrogen in each of the following:



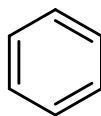
Use the following code to indicate your answers in the box provided:

<b>A</b>	<b>i &gt; ii &gt; iii</b>	<b>D</b>	<b>ii &gt; iii &gt; i</b>
<b>B</b>	<b>i &gt; iii &gt; ii</b>	<b>E</b>	<b>iii &gt; i &gt; ii</b>
<b>C</b>	<b>ii &gt; i &gt; iii</b>	<b>AB</b>	<b>iii &gt; ii &gt; i</b>

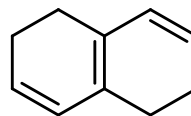
6. The resonance energies of each of the following:



**i**

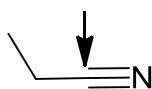


**ii**



**iii**

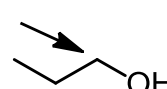
7. The relative oxidation state of the C atom indicated in each of the following:



**i**

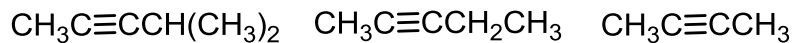


**ii**



**iii**

8. The relative yields of a methyl ketone from the reactions of each of the following with (1)  $\text{BH}_3/\text{THF}$  then (2) aq.  $\text{H}_2\text{O}_2/\text{NaOH}$ :

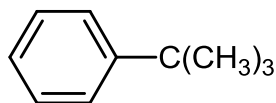


**i**

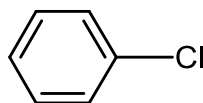
**ii**

**iii**

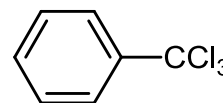
9. The % yield of the *para* product produced by the reaction of  $\text{Br}_2/\text{FeBr}_3$  with each of the following:



**i**

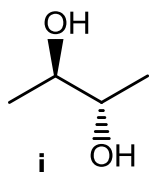


**ii**

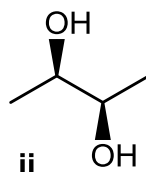


**iii**

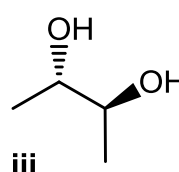
10. The specific rotations of each of the following molecules given that (2R,3R)-butan-2,3-diol has an  $[\alpha]_{\text{D}} = -13.2^\circ$ :



**i**



**ii**

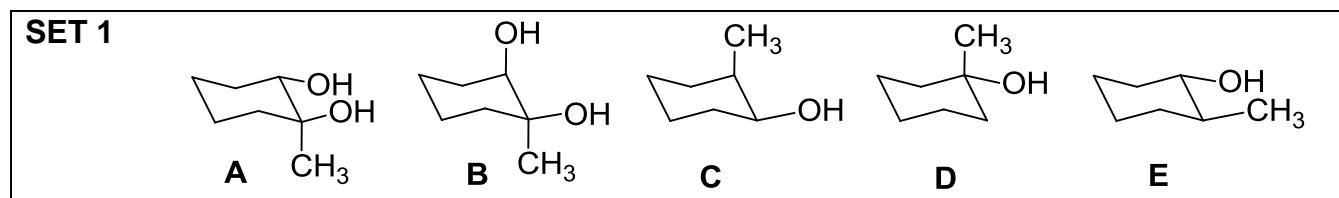


**iii**

**8 % PART 2: STRUCTURE AND PROPERTIES**

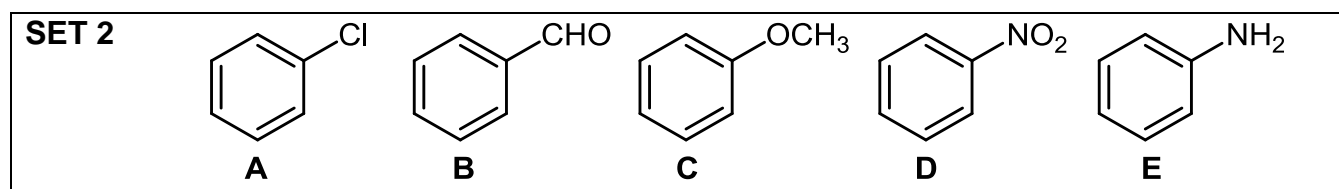
**ANSWER ANY EIGHT (8) OF THE NINE (9) QUESTIONS 11-19.**

**IN SOME CASES more than one answer may be correct and ALL compounds that apply MUST be selected for full credit.**



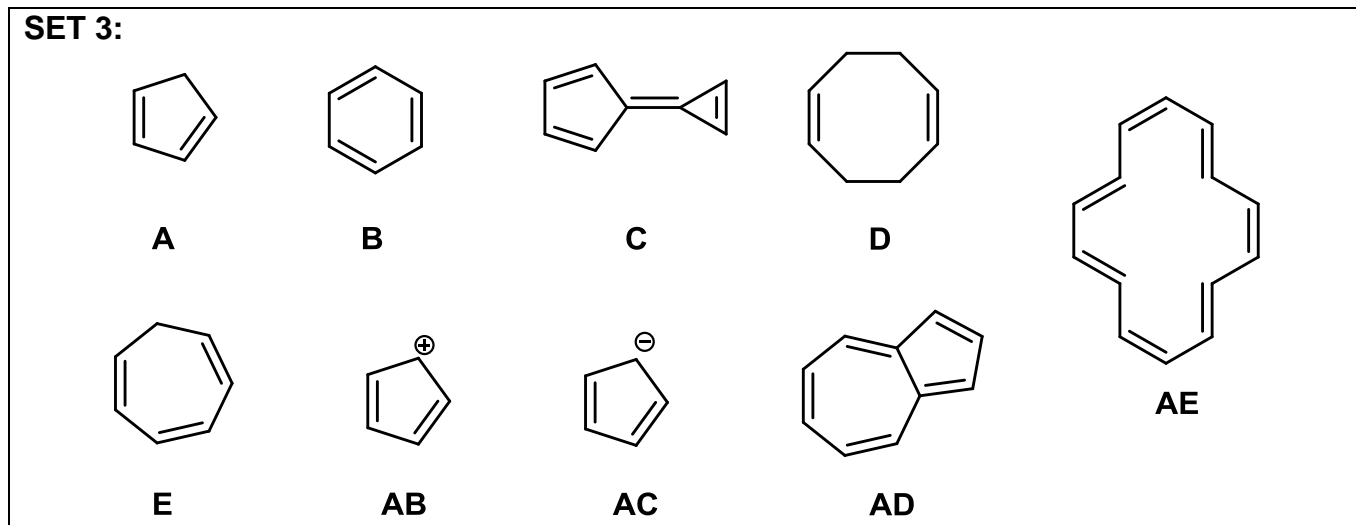
**Answer questions 11-15 by selecting the compounds from SET 1 above.**

- Which compound(s) is (are) optically inactive ?
- Which compound is the **major product** formed from the reaction of 1-methylcyclohexene with (1)  $\text{BH}_3$  then (2) aq.  $\text{H}_2\text{O}_2 / \text{NaOH}$  ?
- Which compound is the **major product** formed from the reaction of 1-methylcyclohexene with aqueous  $\text{H}_2\text{SO}_4$  ?
- Which compound is the **major product** formed from the reaction of 1-methylcyclohexene with (1)  $\text{CH}_3\text{CO}_3\text{H}$  then (2) aq.  $\text{NaOH}$  ?
- Which compound is the **major product** formed from the reaction of 1-methylcyclohexene with  $\text{KMnO}_4$ , aq.  $\text{NaOH}$ ,  $0^\circ\text{C}$  ?



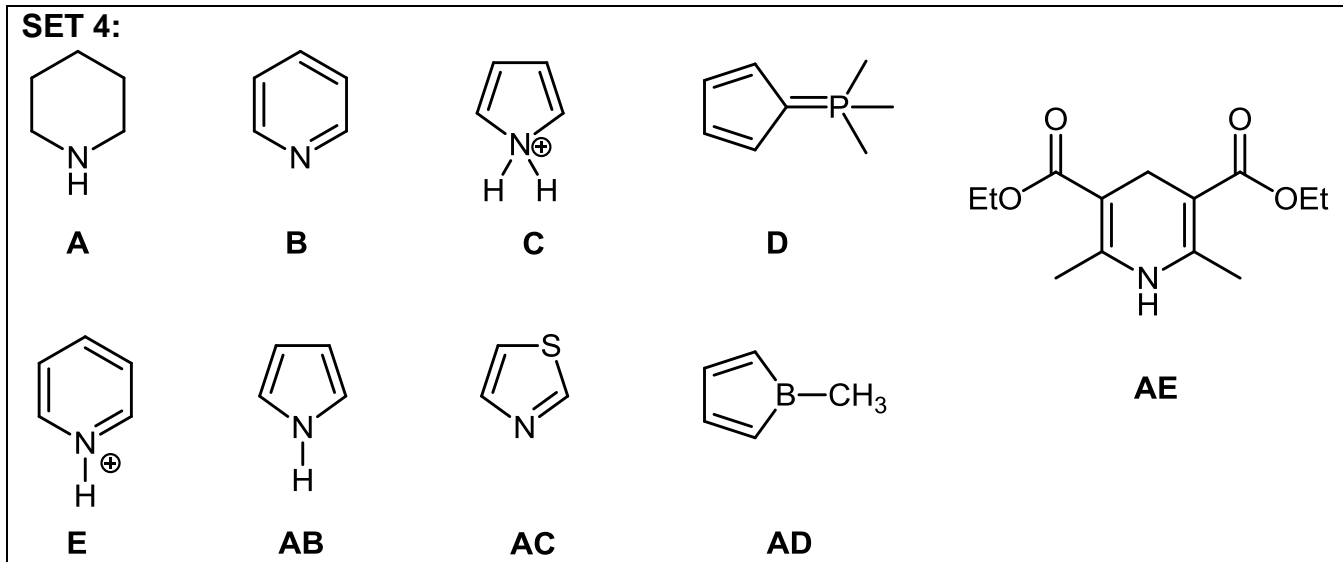
**Answer questions 16-19 about electrophilic aromatic substitution by selecting a compound from SET 2 above**

- Which compound is the **most** activated compared to benzene ?
- Which compound is the **most** deactivated compared to benzene ?
- Which **compound(s)** is/are deactivated and direct *meta* ?
- Which **compound(s)** undergo successful acylation with  $\text{CH}_3\text{C}(=\text{O})\text{Cl} / \text{AlCl}_3$ ?

**9% PART 3: AROMATICITY AND RESONANCE****ANSWER ANY NINE (9) OF THE TEN (10) QUESTIONS 20 - 29.**

Answer questions 20-24 by selecting a SINGLE compound from SET 3 above.

- 20.** Non-aromatic as drawn but has an aromatic conjugate base.
- 21.** Non-aromatic as drawn but has an antiaromatic conjugate base.
- 22.** A diene with no resonance energy stabilization.
- 23.** The compound with the largest "n" value in the Huckel rule
- 24.** An aromatic triene.



Answer questions 25-29 by selecting a SINGLE compound from SET 4 above.

25. Select the compound that contains the **most** acidic proton

26. Select the compound with the **most** basic nitrogen atom

27. Select the compound **most** likely to donate a hydride atom

28. Non aromatic as drawn but has an important aromatic resonance structure

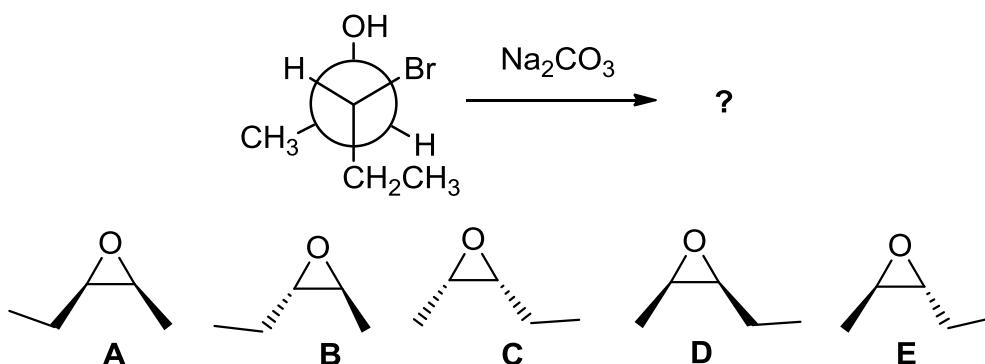
29. An antiaromatic compound.

**16% PART 4: STARTING MATERIALS AND PRODUCTS OF SYNTHESIS**

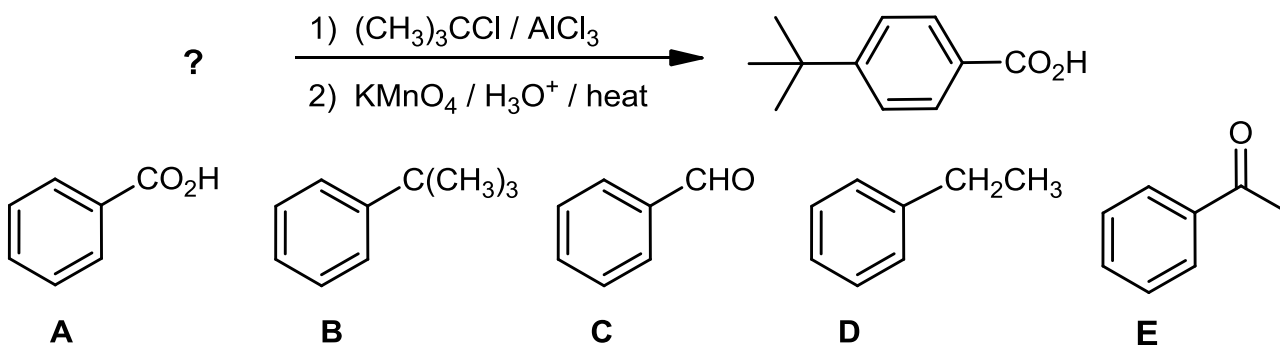
ANSWER ANY EIGHT (8) OF THE NINE (9) QUESTIONS 30-38.

For each of the questions 30 - 38 identify the product(s) obtained or starting material(s) required in order to best complete each of the reaction sequences shown by selecting from the list provided.

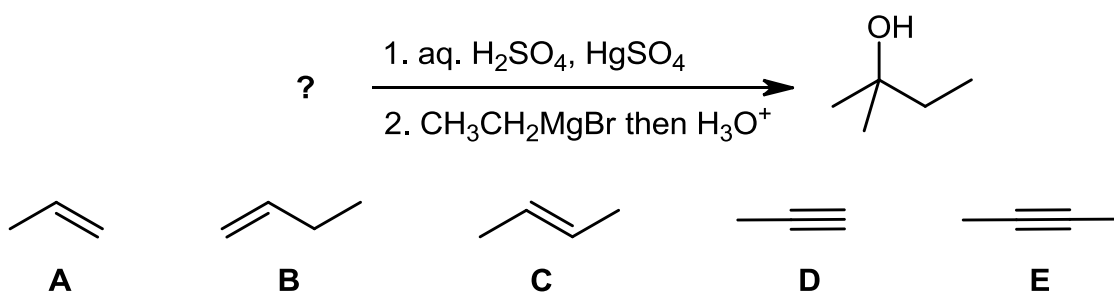
30.



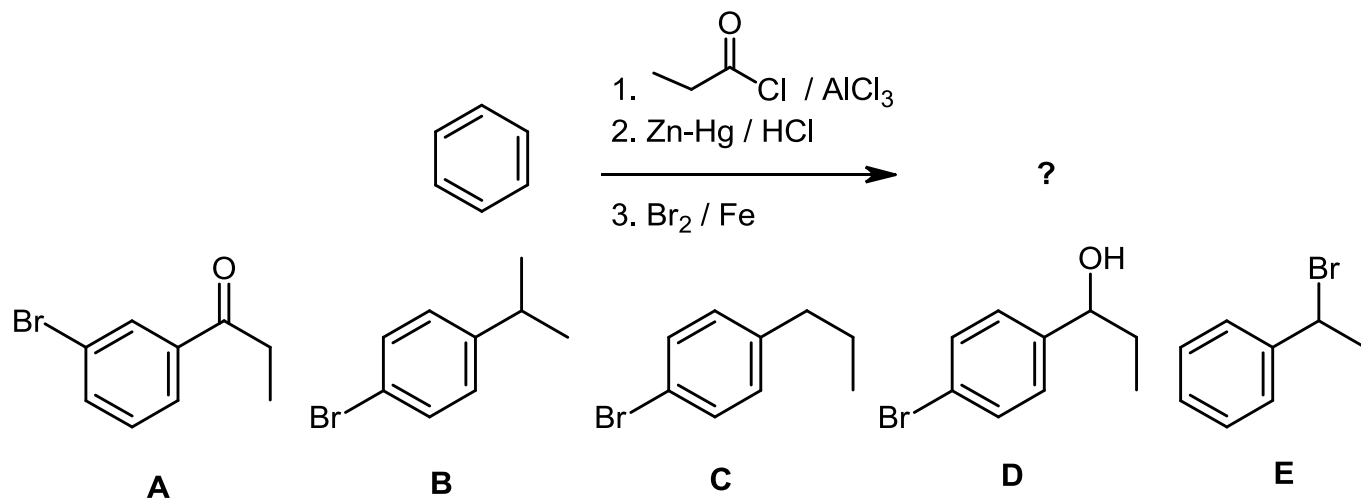
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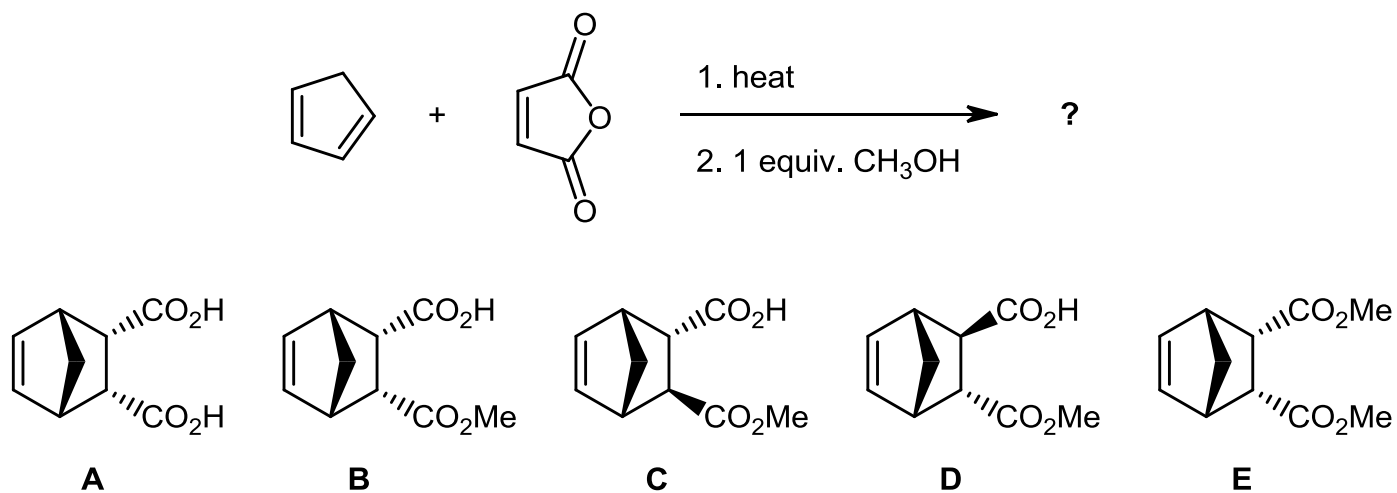
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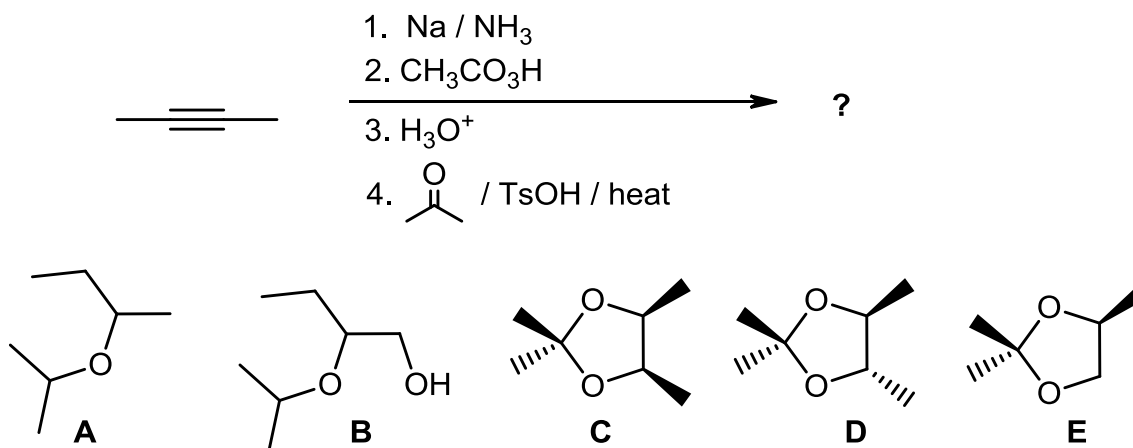
33.



34.

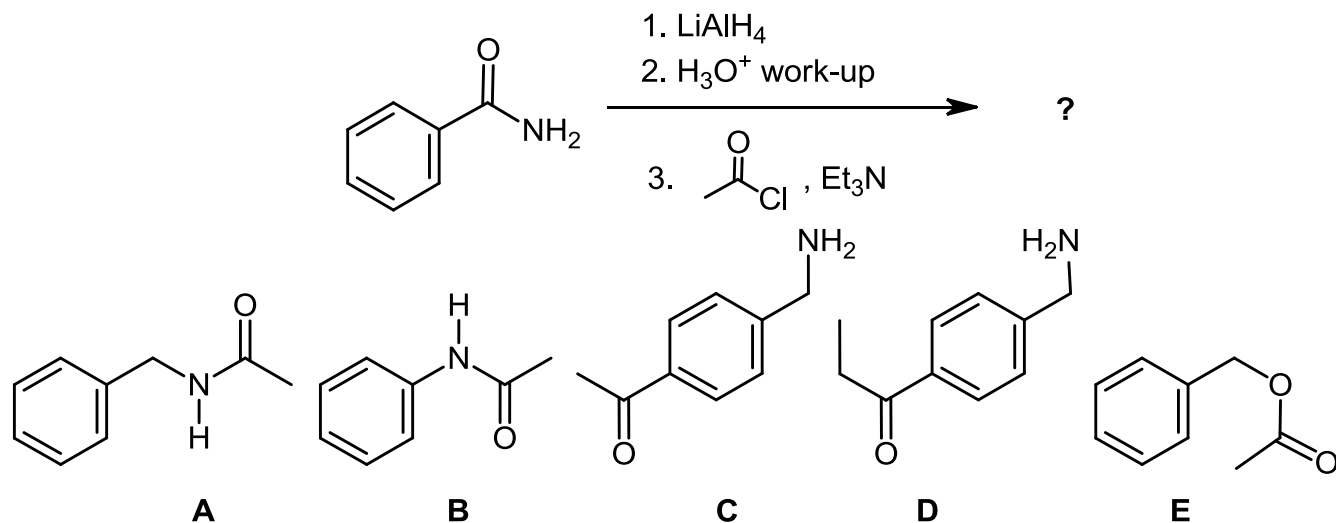


35.

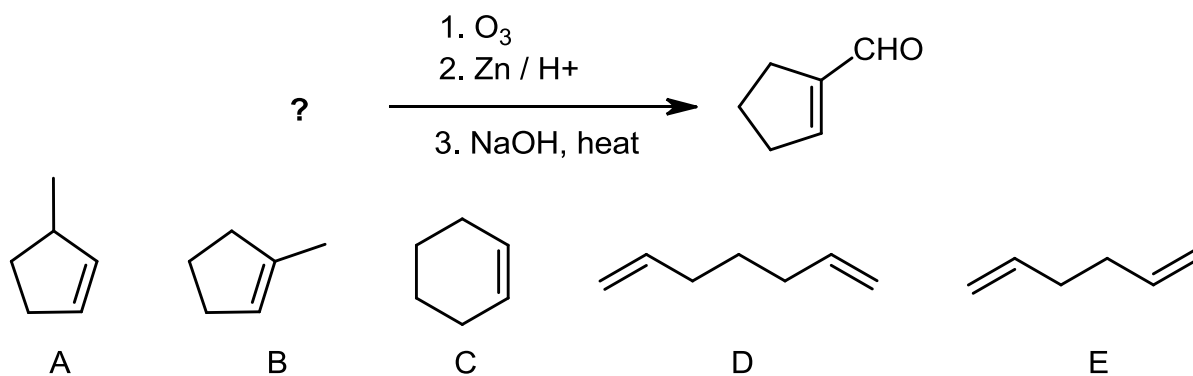




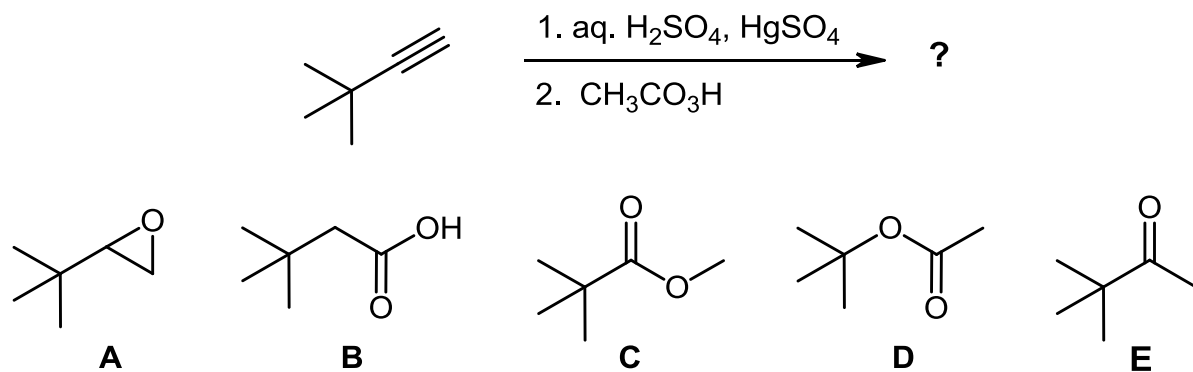
36.



37.

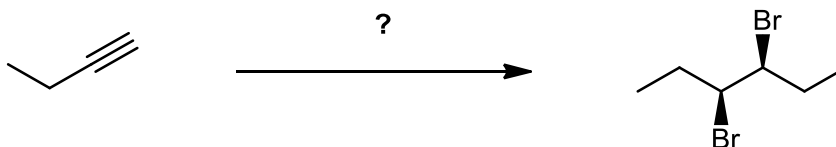


38.



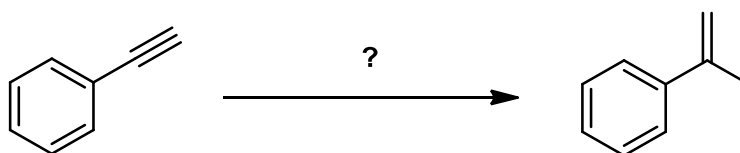
**10% PART 5: REAGENTS FOR SYNTHESIS****ANSWER ANY FIVE (5) OF THE SIX (6) QUESTIONS 39-44**For each of the questions 39-44 identify the reagent(s) required in order to **BEST** complete each of the reaction sequences shown by selecting from the list provided.

39.



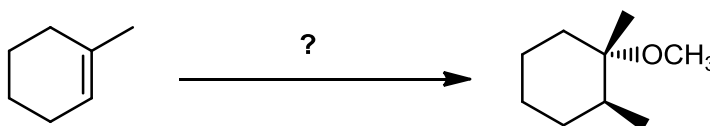
- A. i.  $\text{Br}_2$ , ii.  $\text{NaNH}_2$ ,  $\text{CH}_3\text{CH}_2\text{Br}$ , iii.  $\text{H}_2$ , Pd/C  
 B. i.  $\text{NaNH}_2$ ,  $\text{CH}_3\text{CH}_2\text{Br}$ , ii.  $\text{H}_2$ , Lindlar cat., iii.  $\text{Br}_2$   
 C. i.  $\text{H}_2$ , Lindlar cat., ii.  $\text{NaNH}_2$ ,  $\text{CH}_3\text{CH}_2\text{Br}$ , iii.  $\text{Br}_2$   
 D. i.  $\text{NaNH}_2$ ,  $\text{CH}_3\text{CH}_2\text{Br}$ , ii. Na,  $\text{NH}_3$  iii.  $\text{Br}_2$   
 E. i. Na,  $\text{NH}_3$ , ii.  $\text{NaNH}_2$ ,  $\text{CH}_3\text{CH}_2\text{Br}$ , iii.  $\text{Br}_2$

40.



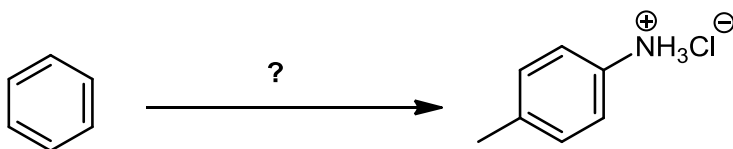
- A. i.  $\text{Hg}(\text{OAc})_2$ ,  $\text{H}_3\text{O}^+$ , ii.  $(\text{Ph})_3\text{P}^+\text{CH}_3$ , NaH  
 B. i. 9-BBN, ii.  $\text{H}_2\text{O}_2$ , aq. NaOH, iii.  $(\text{Ph})_3\text{P}^+\text{CH}_3$ , NaH  
 C. i.  $\text{Hg}(\text{OAc})_2$ ,  $\text{H}_3\text{O}^+$ , ii.  $\text{NaBH}_4$ , iii.  $\text{PCl}_3$ ,  $\text{Et}_3\text{N}$ , iv.  $\text{NaOtBu}$   
 D. i. 9-BBN, ii.  $\text{H}_2\text{O}_2$ , aq. NaOH, iii.  $\text{PCl}_3$ ,  $\text{Et}_3\text{N}$ , iv.  $\text{NaOtBu}$   
 E. i.  $\text{MeMgBr}$ , ii.  $\text{H}_2\text{O}$ ,  $\text{H}_3\text{O}^+$

41.



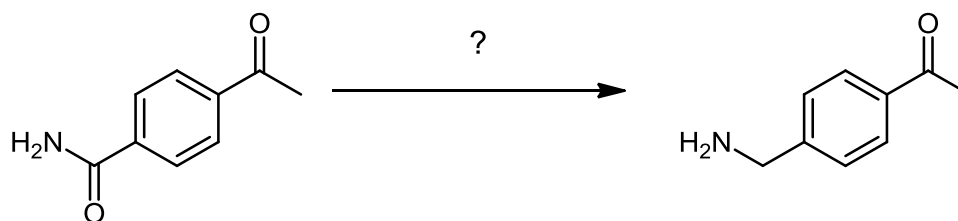
- A. i. MeOH, ii. MeI, NaH  
 B. i. MeI,  $\text{H}_2\text{SO}_4$ , ii. peracetic acid, iii.  $\text{LiAlH}_4$  then  $\text{H}_3\text{O}^+$   
 C. i.  $\text{MeMgBr}$  then  $\text{H}_3\text{O}^+$ , ii. MeOH,  $\text{H}_2\text{SO}_4$   
 D. i. peracetic acid, ii. MeOH,  $\text{H}_2\text{SO}_4$   
 E. i. mCPBA, ii.  $\text{MeMgBr}$  then  $\text{H}_3\text{O}^+$ , iii. MeI, NaH

42.



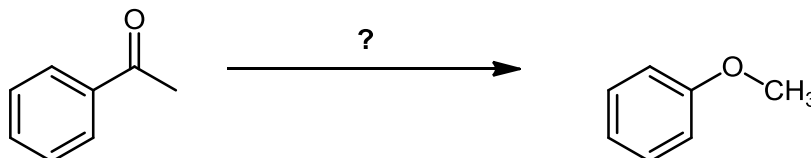
- A. i.  $\text{H}_2\text{SO}_4$ ,  $\text{HNO}_3$ , ii.  $\text{MeCl}$ ,  $\text{AlCl}_3$ , iii.  $\text{Sn}$ ,  $\text{HCl}$   
 B. i.  $\text{NH}_3$ ,  $\text{AlCl}_3$  ii.  $\text{MeCl}$ ,  $\text{AlCl}_3$   
 C. i.  $\text{H}_2\text{SO}_4$ ,  $\text{HNO}_3$ , ii.  $\text{Sn}$ ,  $\text{HCl}$  iii.  $\text{MeCl}$ ,  $\text{AlCl}_3$   
 D. i.  $\text{MeCl}$ ,  $\text{AlCl}_3$ , ii.  $\text{H}_2\text{SO}_4$ ,  $\text{HNO}_3$ , iii.  $\text{Sn}$ ,  $\text{HCl}$   
 E. i.  $\text{MeCl}$ ,  $\text{AlCl}_3$ , ii.  $\text{NH}_3$ ,  $\text{AlCl}_3$

43.



- A.  $\text{H}_2\text{NNH}_2$ ,  $\text{NaOH}$ , heat  
 B. i.  $\text{LiAlH}_4$ , THF then  $\text{H}_3\text{O}^+$ , ii.  $\text{H}_3\text{O}^+$ , heat  
 C. i.  $\text{NaBH}_4$ , ii. PDC, iii.  $\text{H}_3\text{O}^+$   
 D. i.  $\text{HOCH}_2\text{CH}_2\text{OH}$ ,  $\text{TsOH}$ , ii.  $\text{LiAlH}_4$ , THF then  $\text{H}_3\text{O}^+$  iii.  $\text{H}_3\text{O}^+$ , heat  
 E. i.  $\text{Zn}/\text{Hg}$ ,  $\text{HCl}$ , ii.  $\text{NaBH}_4$ ,  $\text{EtOH}$

44.

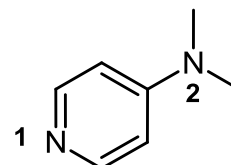


- A. i.  $\text{NaBH}_4$ , ii.  $\text{H}_3\text{O}^+$ , iii.  $\text{H}_2\text{SO}_4$ ,  $\text{MeOH}$   
 B. i.  $\text{MeOH}$ , heat, ii.  $\text{H}_3\text{O}^+$   
 C. i. mCPBA, ii.  $\text{NaOMe}$ ,  $\text{MeOH}$ , heat iii.  $\text{LDA}$ ,  $\text{MeI}$   
 D. i.  $\text{NaBH}_4$ , ii.  $\text{H}_3\text{O}^+$ , iii. mCPBA  
 E. i.  $\text{NaBH}_4$ , ii.  $\text{LDA}$ ,  $\text{MeI}$ , iii. mCPBA

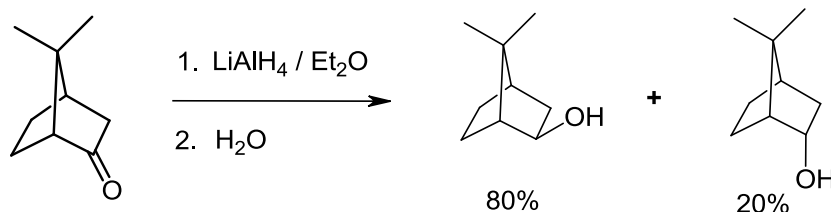
**10% PART 6: EXPLANATION OF PHENOMENA****ANSWER ALL FIVE (5) OF THE QUESTIONS 45 - 49.****Choose the single explanation that best rationalises the phenomenon indicated.**

45. Dimethylaminopyridine has two basic nitrogen atoms labeled as **1** and **2** (shown below). Which N atom is more basic and why ?

- A. N1 because the N1 lone pair is in an  $sp^2$  hybrid orbital  
 B. N1 because the N1 lone pair is in a p orbital  
 C. N1 because its conjugate acid is resonance stabilised  
 D. N2 because the N2 lone pair is in an  $sp^3$  hybrid orbital  
 E. N2 because its conjugate acid is resonance stabilised  
 AB. N2 because the N2 lone pair is in an  $sp^2$  hybrid orbital



46. The following ketone reacts with  $LiAlH_4$  with the stereoselectivity shown below. This is because:



- A. Substituents tend to prefer equatorial positions on cyclohexane ring systems  
 B. Polar substituents tend to prefer axial positions on cyclohexane ring systems  
 C. There is less steric hindrance if the nucleophile attacks from the top face  
 D. There is less steric hindrance if the nucleophile attacks from the bottom face  
 E. There is less steric hindrance if the electrophile attacks from the top face  
 AB. There is less steric hindrance if the electrophile attacks from the bottom face

47. Consider the reaction of bromobenzene with  $\text{HNO}_3 / \text{H}_2\text{SO}_4$ . Which isomer of bromonitrobenzene is the major product and why ?

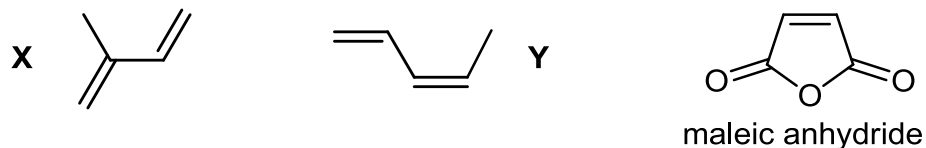
- A. ortho because the  $-\text{NO}_2$  group is activating and o,p-directing
- B. meta because the  $-\text{NO}_2$  group is deactivating and m-directing
- C. para due to steric effects and because the  $-\text{NO}_2$  is activating and o,p-directing
- D. ortho because the  $-\text{Br}$  group is activating and o,p-directing
- E. meta because the  $-\text{Br}$  group is deactivating and m-directing
- AB.** para due to steric effects and because the  $-\text{Br}$  is deactivating and o,p-directing

48. Two carboxylic acid derivatives (an amide and an ester) are shown below. Which is more acidic and why ?



- A. The ester because the conjugate base is better stabilized by resonance
- B. The ester due to the electron donating effect of the methoxy group
- C. The ester due to the electronegativity of the O atom
- D. The amide due to the electronegativity of the N atom
- E. The amide due to the electron donating effect of the amino group
- AB.** The amide because the conjugate base is better stabilized by resonance

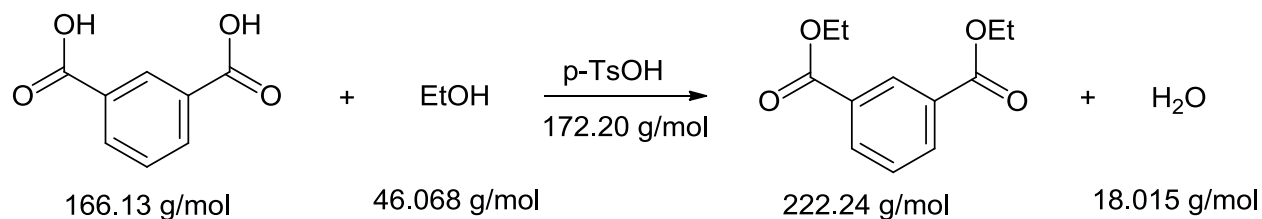
49. Which of the following reacts faster with maleic anhydride and why ?



- A. **X** because it has an electron donating substituent that activates it
- B. **X** because it has an electron withdrawing substituent that activates it
- C. **X** because the reactive conformation of **Y** is destabilised
- D. **Y** because it has an electron donating substituent that activates it
- E. **Y** because it has an electron withdrawing substituent that activates it
- AB.** **Y** because the reactive conformation of **X** is destabilised

**5% PART 7: LABORATORY****WRITE YOUR ANSWERS IN THE BLUE ANSWER BOOKLET PROVIDED.**

Calculate the % yield of the ester product (show your working) based on the following experimental data.



Densities: ethanol = 0.79 g/mL, chloroform = 1.56 g/mL, ethyl ethanoate = 0.90 g/mL

m-Phthalic acid (1.66 g) and anhydrous ethanol (1.50 mL) were mixed in anhydrous chloroform (5.0 mL), and a few crystals of p-tosic acid were added. After heating the solution for 3 hours at 50 °C, the reaction mixture was cooled and evaporated to dryness. The crude solid mixture was dissolved in ethyl ethanoate (15 mL), and the solution was washed with 10% NaHCO<sub>3</sub> (15 mL), 2M HCl (15 mL), and then dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After filtration, the organic solution was evaporated on a rotary evaporator and dried under high vacuum to afford diethyl phthalate as a colorless oil (1.111 g).

**8% PART 8: MECHANISM**

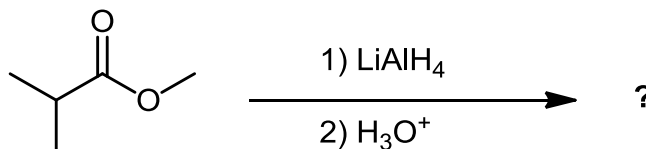
ANSWER TWO (2) QUESTIONS, ONE FROM PART A AND ONE FROM PART B.

WRITE YOUR ANSWERS IN THE BLUE ANSWER BOOKLET PROVIDED.

NO REAGENTS OTHER THAN THOSE ALREADY SHOWN IN EACH QUESTION ARE REQUIRED.

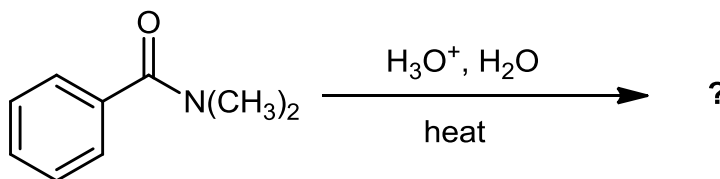
(4) PART A: Draw the curly arrow mechanism for ONE of the following transformations:

i.



OR

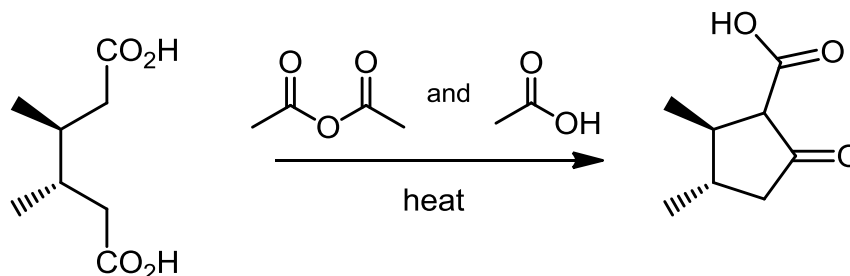
ii.



(4) PART B : Draw the curly arrow mechanism for ONE of the following transformations:

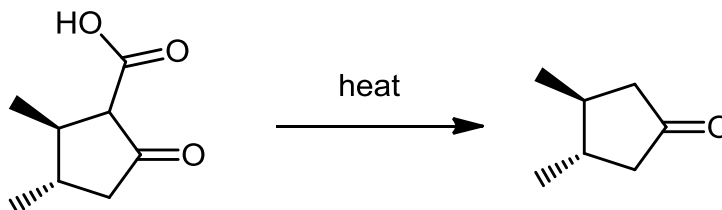
The Blanc cyclization is a method to rapidly prepare cyclic ketones from di-acids applying chemistry we have learned in Chem 353.

i. Provide a mechanism for the first part of the Blanc reaction shown below:



OR

ii. Provide a mechanism for the second part of the Blanc reaction shown below:

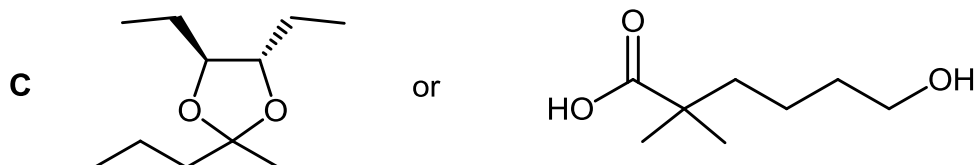
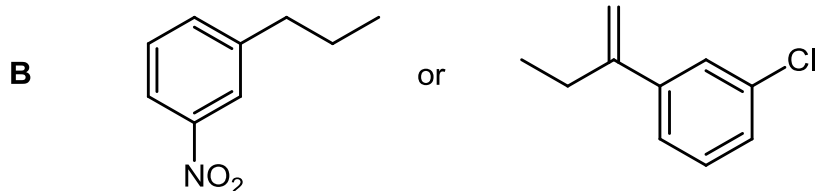
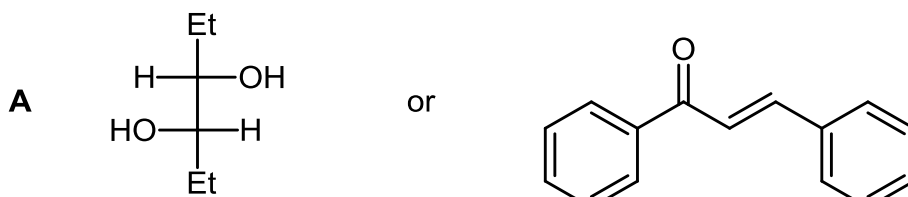


**12% PART 9: TOTAL SYNTHESIS**

WRITE YOUR ANSWERS IN THE BLUE ANSWER BOOKLET PROVIDED.

Design an efficient synthesis from the starting materials in the list below for THREE (3) of the following target molecules. Choose ONE target from each of the three sections A, B and C. DO NOT SHOW MECHANISMS (*i.e.* curly arrows are NOT required)

SHOW YOUR ANSWER AS A STEPWISE REACTION SCHEME SHOWING THE REAGENT REQUIRED FOR EACH STEP AND THE SYNTHETIC INTERMEDIATE FORMED FROM EACH REACTION.



**Permitted Materials and Reagents**

**NOTE:** any materials that contribute carbon atoms to the target molecule must come from this allowed list:

- any organic compounds with no more than **FOUR** carbons
- benzene
- cyclohexanol
- You can use any solvents or other reagents for the reactions provided that they do not contribute carbon atoms to the target.



**10% PART 10: STRUCTURE DETERMINATION****WRITE YOUR ANSWERS IN THE BLUE ANSWER BOOKLET PROVIDED**

Compound **A** ( $C_{12}H_{22}O$ ) is an achiral compound and a constituent of the sex pheromone of the common cutworm. After refluxing **A** in aq. NaOH and dilute aq. acid work up, two new compounds were obtained, ethanoic acid and **B**,  $C_{10}H_{20}O$ .

Compound **B** was then treated with pyridinium chlorochromate (PCC) in methylene chloride to give **C**. **C** gave a yellow precipitate when tested with 2,4-dinitrophenylhydrazine and a deposit of silver in the Tollen's test. **C** was then reduced with  $NH_2NH_2$  / ethylene glycol / heat to give **D**,  $C_{10}H_{20}$ . Reaction of **D** with  $KMnO_4$  / aq. NaOH at  $0^\circ C$  gave **E**, a meso diol,  $C_{10}H_{22}O_2$ .

Alternatively, **B** was reacted with ozone followed by work-up with  $H_2O_2$  to give two new compounds **F**,  $C_5H_{10}O_2$  and **G**,  $C_5H_{10}O_3$ . Compound **G** was observed to readily lose water to give **H**,  $C_5H_8O_2$  which was found to be identical to the compound formed when cyclopentanone was reacted with  $CH_3CO_3H$ . The identity of compound **F** was confirmed by independent synthesis: diethyl malonate (also known as diethyl propanedioate) was reacted with sodium ethoxide in ethanol and then 1-bromopropane with added catalytic NaI. Hydrolysis of the resulting product by heating with aq. NaOH and then acidification / heat resulted in the evolution of a gas and the formation of **F**.

**Identify the compounds A to H showing any relevant stereochemistry (drawn structures are sufficient).**

**\*\*\*THE END\*\*\***

IRH / DD W2019

## PERIODIC TABLE

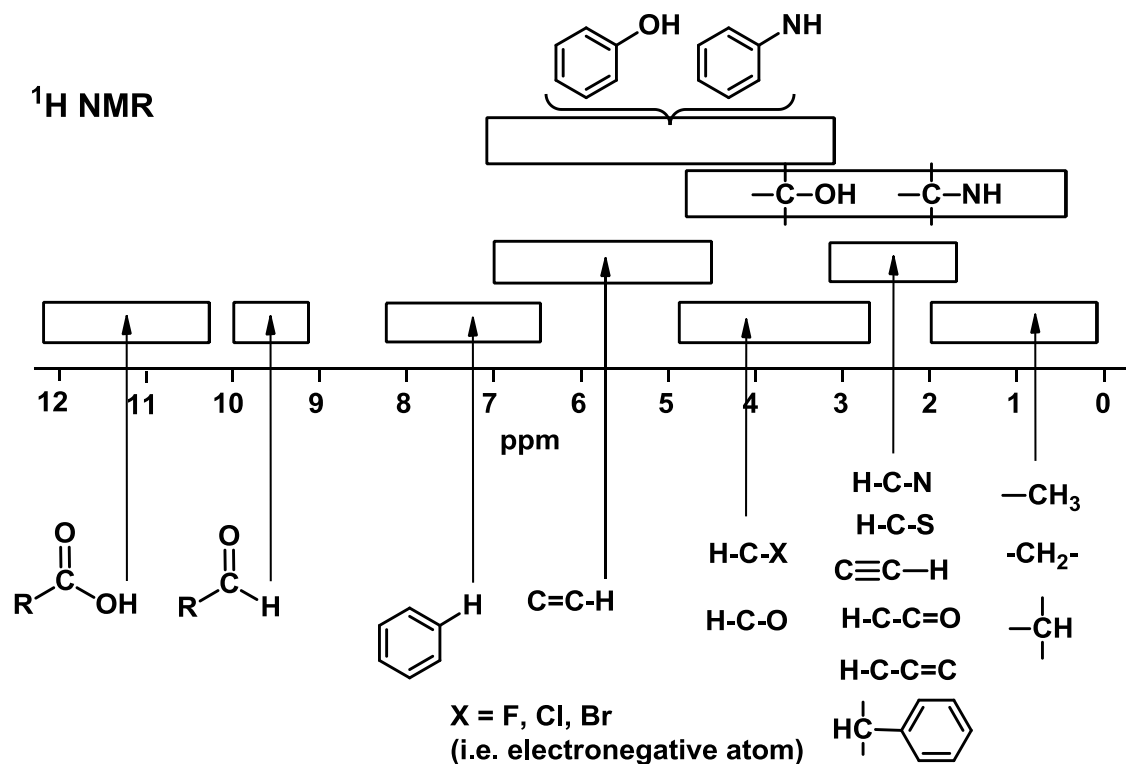
<b>1</b>																<b>18</b>	
<b>1A</b>											<b>13</b>	<b>14</b>	<b>15</b>	<b>16</b>	<b>17</b>	<b>8A</b>	
1 <b>H</b> 1.008	<b>2</b> 2A											<b>3A</b>	<b>4A</b>	<b>5A</b>	<b>6A</b>	<b>7A</b>	2 <b>He</b> 4.003
3 <b>Li</b> 6.941	4 <b>Be</b> 9.012											5 <b>B</b> 10.81	6 <b>C</b> 12.01	7 <b>N</b> 14.01	8 <b>O</b> 16.00	9 <b>F</b> 19.00	10 <b>Ne</b> 20.18
11 <b>Na</b> 22.99	12 <b>Mg</b> 24.31	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>	<b>9</b>	<b>10</b>	<b>11</b>	<b>12</b>	13 <b>Al</b> 26.98	14 <b>Si</b> 28.09	15 <b>P</b> 30.97	16 <b>S</b> 32.07	17 <b>Cl</b> 35.45	18 <b>Ar</b> 39.95
19 <b>K</b> 39.10	20 <b>Ca</b> 40.08	21 <b>Sc</b> 44.96	22 <b>Ti</b> 47.88	23 <b>V</b> 50.94	24 <b>Cr</b> 52.00	25 <b>Mn</b> 54.94	26 <b>Fe</b> 55.85	27 <b>Co</b> 58.93	28 <b>Ni</b> 58.69	29 <b>Cu</b> 63.55	30 <b>Zn</b> 65.38	31 <b>Ga</b> 69.72	32 <b>Ge</b> 72.59	33 <b>As</b> 74.92	34 <b>Se</b> 78.96	35 <b>Br</b> 79.90	36 <b>Kr</b> 83.80
37 <b>Rb</b> 85.47	38 <b>Sr</b> 87.62	39 <b>Y</b> 88.91	40 <b>Zr</b> 91.22	41 <b>Nb</b> 92.91	42 <b>Mo</b> 95.94	43 <b>Tc</b> (98)	44 <b>Ru</b> 101.1	45 <b>Rh</b> 102.9	46 <b>Pd</b> 106.4	47 <b>Ag</b> 107.9	48 <b>Cd</b> 112.4	49 <b>In</b> 114.8	50 <b>Sn</b> 118.7	51 <b>Sb</b> 121.8	52 <b>Te</b> 127.6	53 <b>I</b> 126.9	54 <b>Xe</b> 131.3
55 <b>Cs</b> 132.9	56 <b>Ba</b> 137.3	57* <b>La</b> 138.9	72 <b>Hf</b> 178.5	73 <b>Ta</b> 180.9	74 <b>W</b> 183.9	75 <b>Re</b> 186.2	76 <b>Os</b> 190.2	77 <b>Ir</b> 192.2	78 <b>Pt</b> 195.1	79 <b>Au</b> 197.0	80 <b>Hg</b> 200.6	81 <b>Tl</b> 204.4	82 <b>Pb</b> 207.2	83 <b>Bi</b> 209.0	84 <b>Po</b> (209)	85 <b>At</b> (210)	86 <b>Rn</b> (222)
87 <b>Fr</b> (223)	88 <b>Ra</b> 226.0	89** <b>Ac</b> (227)	104 <b>Rf</b> (261)	105 <b>Ha</b> (262)	106 <b>Sg</b> (263)	107 <b>Ns</b> (262)	108 <b>Hs</b> (265)	109 <b>Mt</b> (266)	110 <b>Uun</b> (269)	111 <b>Uuu</b> (272)							

**Lanthanides \***

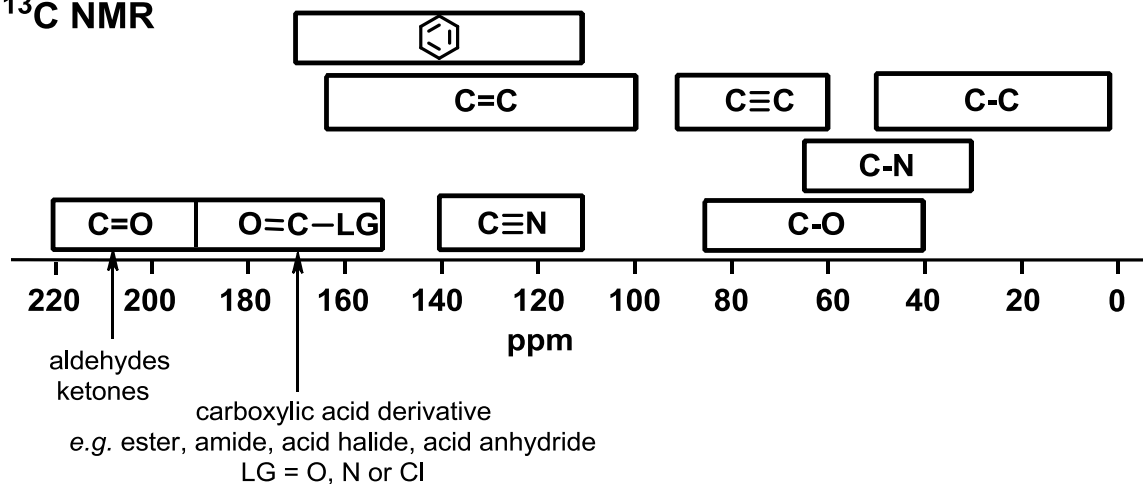
58 <b>Ce</b> 140.1	59 <b>Pr</b> 140.9	60 <b>Nd</b> 144.2	61 <b>Pm</b> (145)	62 <b>Sm</b> 150.4	63 <b>Eu</b> 152.0	64 <b>Gd</b> 157.3	65 <b>Tb</b> 158.9	66 <b>Dy</b> 162.5	67 <b>Ho</b> 164.9	68 <b>Er</b> 167.3	69 <b>Tm</b> 168.9	70 <b>Yb</b> 173.0	71 <b>Lu</b> 175.0
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**Actinides \*\***

90 <b>Th</b> 232.0	91 <b>Pa</b> 231.0	92 <b>U</b> 238.0	93 <b>Np</b> 237.0	94 <b>Pu</b> (244)	95 <b>Am</b> (243)	96 <b>Cm</b> (247)	97 <b>Bk</b> (247)	98 <b>Cf</b> (251)	99 <b>Es</b> (252)	100 <b>Fm</b> (257)	101 <b>Md</b> (258)	102 <b>No</b> (259)	103 <b>Lr</b> (260)
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**SPECTROSCOPIC TABLES** **$^1\text{H}$  NMR CHARACTERISTIC CHEMICAL SHIFTS / ppm**

	R = methyl	methylene	methyne	other	
$\text{R}-\text{C}-\text{H}$	$-\text{CH}_3$ 0.9	$-\text{CH}_2-$ 1.4	$-\text{CH}$ 1.5	$\text{sp}^3\text{C}-\text{OH}$	1-5
$\text{R}-\text{C}=\text{C}-\text{H}$	1.6	2.3	2.6	$\text{sp}^3\text{C}-\text{NH}$	1-3
$\text{R}-\text{C}(=\text{O})-\text{H}$	2.1	2.4	2.5	$\text{C}\equiv\text{CH}$	2.5
$\text{R}-\text{N}-\text{H}$	2.2	2.5	2.9	$\text{C}=\text{C}-\text{H}$	4.5-6.5
$\text{R}-\text{C}_6\text{H}_5$	2.3	2.7	3.0	$\text{H}-\text{C}_6\text{H}_5$	6.5-8
$\text{R}-\text{Br}$	2.7	3.3	4.1	$\text{R}-\text{C}(=\text{O})-\text{H}$	9-10
$\text{R}-\text{Cl}$	3.1	3.4	4.1	$\text{R}-\text{C}(=\text{O})-\text{OH}$	9-12
$\text{R}-\text{O}-\text{H}$	3.3	3.4	3.7		

**$^{13}\text{C}$  NMR** **$^{13}\text{C}$  NMR CHARACTERISTIC CHEMICAL SHIFTS / ppm**

$\text{—CH}_3$ 0-30	$\text{>CH}_2$ 10-50	$\text{—}\overset{\text{ }}{\underset{\text{ }}{\text{C}}}\text{—H}$ 25-60	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—O—}$ 155-180
$\text{—C}\equiv\text{C—}$ 65-90	$\text{>C=C<}$ 80-145	$\text{—}\overset{\text{ }}{\underset{\text{ }}{\text{C}}}\text{—Br}$ 10-40	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—OH}$ 160-185
 110-170	$\text{—}\overset{\text{ }}{\underset{\text{ }}{\text{C}}}\text{—Cl}$ 20-50	$\text{—}\overset{\text{ }}{\underset{\text{ }}{\text{C}}}\text{—OH}$ 45-75	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—H}$ 190-210
	$\text{—}\overset{\text{ }}{\underset{\text{ }}{\text{C}}}\text{—N}$ 30-65	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—}$ 190-220	$\text{—C}\equiv\text{N}$ 110-140

**INFRA-RED GROUP ABSORPTION FREQUENCIES**

	<u>TYPE OF VIBRATION</u>	<u>FREQUENCY (cm<sup>-1</sup>)</u>	<u>WAVELENGTH (μ)</u>	<u>INTENSITY (1)</u>	
C-H	Alkanes (stretch)	3000-2850	3.33-3.51	s	
	-CH <sub>3</sub> (bend)	1450 and 1375	6.90 and 7.27	m	
	-CH <sub>2</sub> - (bend)	1465	6.83	m	
	Alkenes	(stretch)	3100-3000	3.23-3.33	m
		(bend)	1700-1000	5.88-10.0	s
	Aromatics	(stretch)	3150-3050	3.17-3.28	s
		(out-of-plane bend)	1000-700	10.0-14.3	s
	Alkyne (stretch)	ca. 3300	ca.3.03	s	
	Aldehyde		2900-2800	3.45-3.57	w
			2800-2700	3.57-3.70	w
C-C	Alkane	not usually useful			
C=C	Alkene	1680-1600	5.95-6.25	m-w	
	Aromatic	1600-1400	6.25-7.14	m-w	
C≡C	Alkyne	2250-2100	4.44-4.76	m-w	
C=O	Aldehyde	1740-1720	5.75-5.81	s	
	Ketone	1725-1705	5.80-5.87	s	
	Carboxylic acid	1725-1700	5.80-5.88	s	
	Ester	1750-1730	5.71-5.78	s	
	Amide	1700-1640	5.88-6.10	s	
	Anhydride		ca. 1810	ca. 5.52	s
			ca. 1760	ca. 5.68	s
	Acyl chloride	1800	5.55	s	
C-O	Alcohols, Ethers, Esters,				
	Carboxylic acids	1300-1000	7.69-10.0	s	
O-H	Alcohols, Phenols				
	Free	3650-3600	2.74-2.78	m	
	H-Bonded	3400-3200	2.94-3.12	m	
	Carboxylic acids (2)	3300-2500	3.03-4.00	m	
N-H	Primary and secondary amines	ca. 3500	ca. 2.86	m	
C≡N	Nitriles	2260-2240	4.42-4.46	m	
N=O	Nitro (R-NO <sub>2</sub> )	1600-1500	6.25-6.67	s	
		1400-1300	7.14-7.69	s	
C-X	Fluoride	1400-1000	7.14-10.0	s	
	Chloride	800-600	12.5-16.7	s	
	Bromide, Iodide	<600	>16.7	s	

(1) s = strong, m = medium and w = weak

(2) note that the -OH absorption of solid carboxylic acids run as a nujol mull can be difficult to see as they may be very broad.