

UNIVERSITY OF CALGARY

FACULTY OF SCIENCE

FINAL EXAMINATION

CHEMISTRY 353

April 24th, 2012

Time: 3 Hours

PLEASE WRITE YOUR **NAME, STUDENT I.D. NUMBER** ON THE **COMPUTER ANSWER SHEET** AND THE **BOOKLET** FOR THE WRITTEN ANSWER QUESTIONS.

**READ THE INSTRUCTIONS CAREFULLY**

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 examination booklet. Parts 1 - 6 consist of a series of multiple choice questions numbered 1 - 55 which are to be answered on your computer 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 are permitted during the exam; calculators are also permitted, but NOT programmable calculators.

**Absolutely no other electronic devices are allowed.**

Value

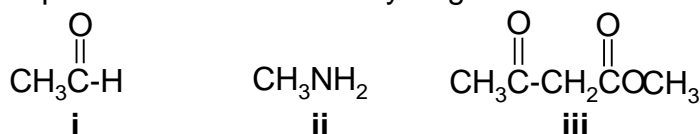
12%

**PART 1: RELATIVE PROPERTIES****ANSWER ANY EIGHT (8) OF QUESTIONS 1-10.**

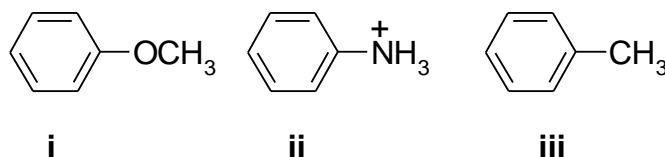
Arrange the items in questions 1-10 in **DECREASING ORDER** (*i.e.* greatest, most etc. first) with respect to the indicated property. Use the following code to indicate your answers in the box provided:

<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>

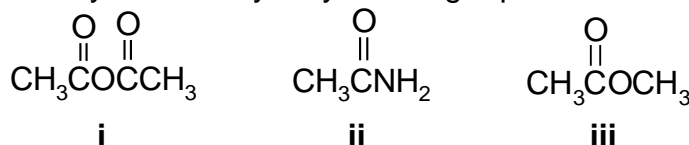
1. The relative pKa of the most acidic hydrogen in each of the following:



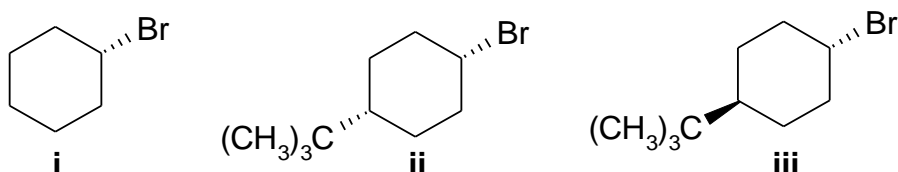
2. The relative rate of reaction of  $\text{Br}_2 / \text{FeBr}_3$  with each of the following:



3. The relative reactivity towards hydrolysis using aqueous NaOH of the following:



4. The relative reactivity of the following when heated with potassium *tert*-butoxide



5. The number of enolisable (or  $\alpha$ -protons) in each of the following:

<b>i</b> 2-pentanone	<b>ii</b> benzaldehyde	<b>iii</b> ethyl ethanoate
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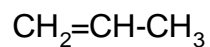
Use the following code to indicate your answers in the box provided:

- |          |                           |           |                           |
|----------|---------------------------|-----------|---------------------------|
| <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> |

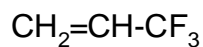
6. The relative stability of the carbocations formed by the reaction of each of the following with  $\text{H}_2\text{SO}_4$ :



**i**

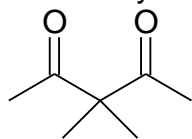


**ii**

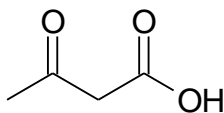


**iii**

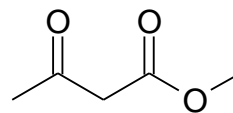
7. The relative acidity of the most acidic H in each of the following :



**i**

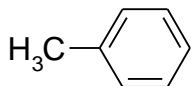


**ii**

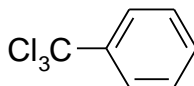


**iii**

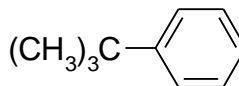
8. The % yield of the para product produced by the reaction of  $\text{HNO}_3 / \text{H}_2\text{SO}_4$  with each of the following:



**i**

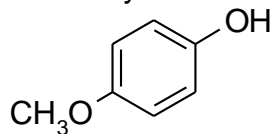


**ii**

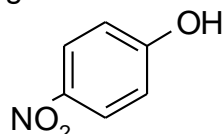


**iii**

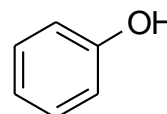
9. The relative acidity of the following:



**i**

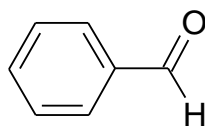


**ii**

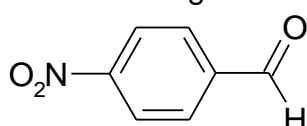


**iii**

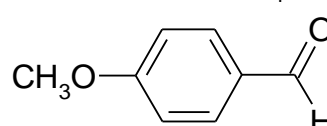
10. The relative reactivity of the following towards reaction with  $\text{NaBH}_4$ :



**i**



**ii**

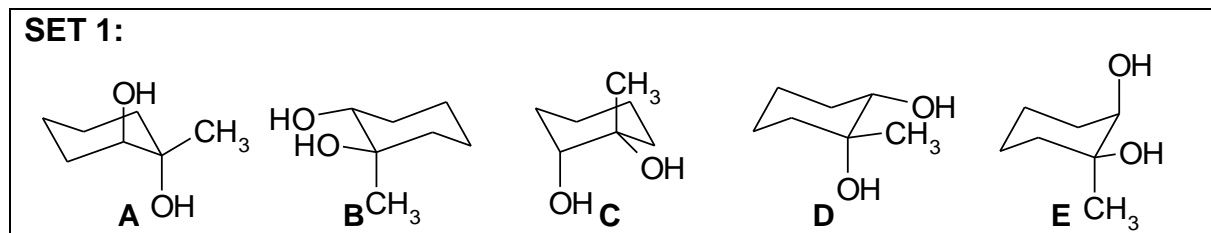


**iii**

Value

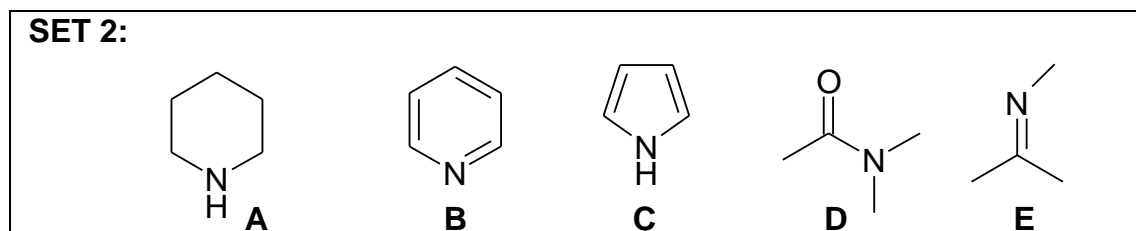
**10% PART 2: STRUCTURE AND PROPERTIES****ANSWER ANY TEN (10) OF THE ELEVEN (11) QUESTIONS 11-21.**

In some cases more than one answer may be correct and **ALL** compounds that apply **MUST** be selected for full credit.



Answer questions 11-14 by selecting the compounds from SET 1 above.

- Select **TWO** structures that show an axial methyl group.
- Select **A SINGLE** compound that has –OH groups that are *trans* and at least one –OH is equatorial
- Select **TWO** structures that are the result of the reaction of 1-methylcyclohexene with cold alkaline potassium permanganate.
- Select **A SINGLE** compound that could have been made via an anti addition of two –OH groups to 1-methylcyclohexene.

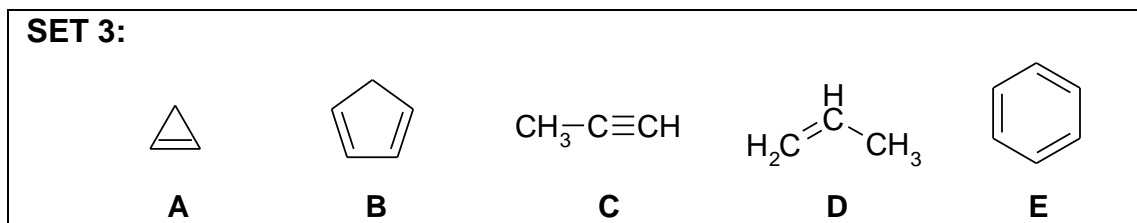


Answer questions 15-16 by selecting the compounds from SET 2 above.

- Select **ALL** the structures contain N atoms that are  $sp^2$  hybridised.
- Select **ALL** the structures whose conjugate acids contain N atoms that are  $sp^2$  hybridised.

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**SET 3:**

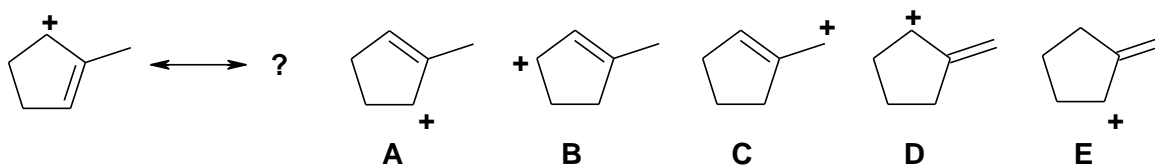


Answer questions 17-19 by selecting the compounds from SET 3 above.

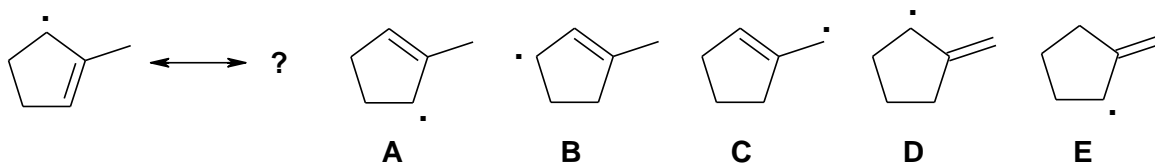
17. Select the structure that has the **lowest** pKa.
18. Select the structure that gives the **most** stable carbocation when reacted with  $\text{H}^+$ .
19. Select the structure that has the **most** types of hydrogen.

Answer questions 20-21 by selecting the compounds from the answers provided.

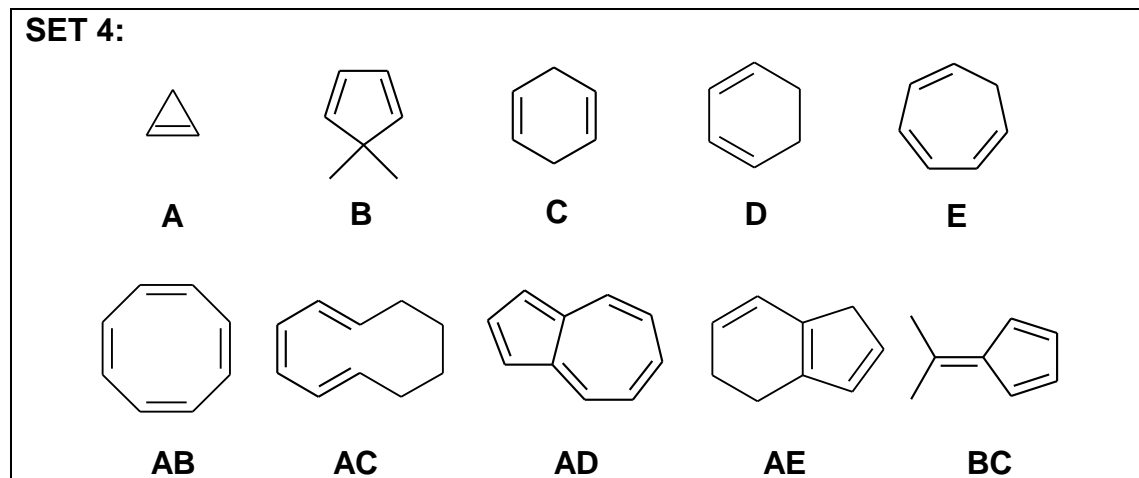
20. Which of the following systems are resonance contributors of the carbocation shown below ? (select all that apply)



21. Which of the following systems are resonance contributors of the radical shown below ? (select all that apply)



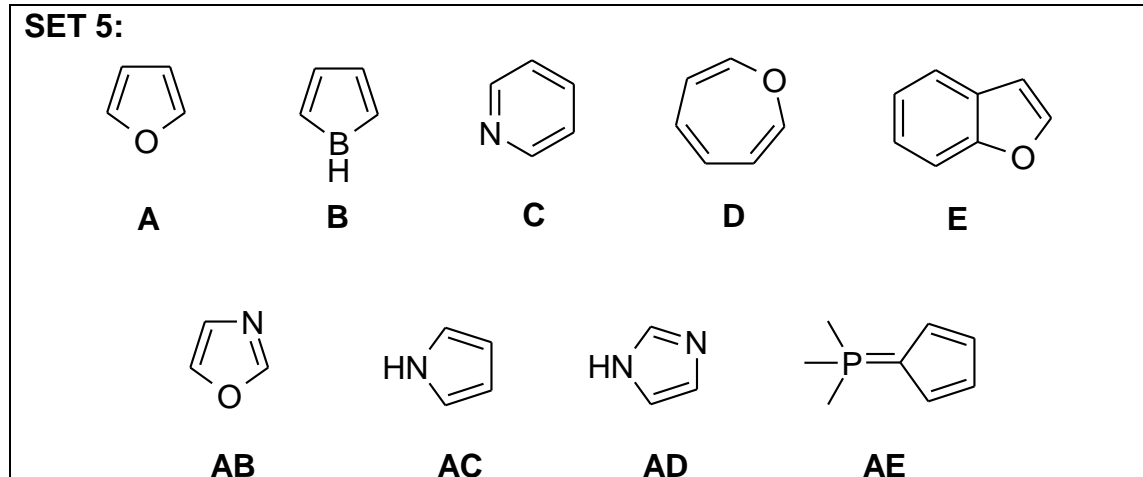
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**9% PART 3: AROMATICITY AND RESONANCE****ANSWER NINE (9) OF THE TEN (10) QUESTIONS 22 - 31.**

Answer questions 22-26 by selecting a single compound from SET 4 above.

22. An aromatic compound.
23. Non-aromatic as drawn, but has an important aromatic resonance contributor.
24. Non-aromatic as drawn, but has an aromatic conjugate base.
25. A non-conjugated polyene.
26. The compound with no resonance energy stabilization.

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Answer questions 27-31 by selecting a single compound from SET 5 above.

27. An aromatic system that has a non-aromatic conjugate acid.

28. Aromatic as drawn and has an aromatic tautomer.

29. Non-aromatic as drawn but has an important aromatic resonance structure.

30. An anti-aromatic system as drawn where  $n=1$  in the Huckel rule.

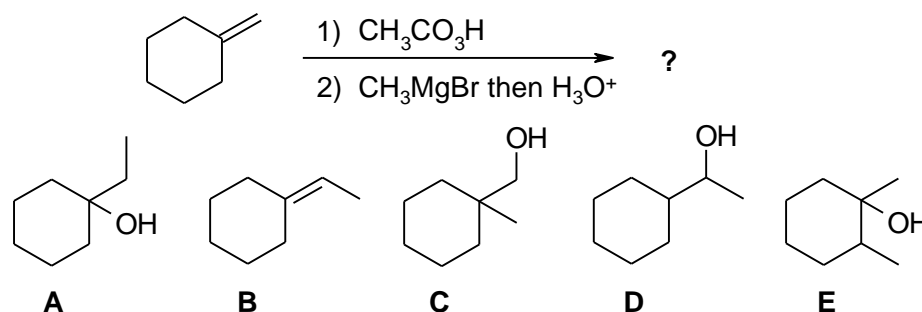
31. An aromatic compound where  $n = 2$  in the Huckel rule.

Value

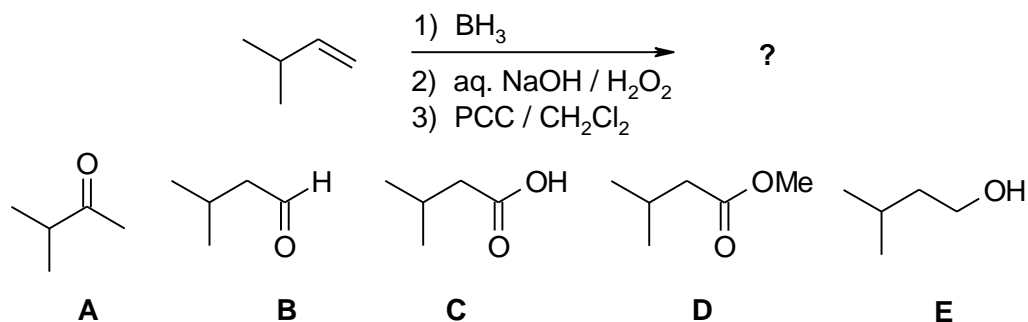
**16% PART 4: STARTING MATERIALS AND PRODUCTS OF SYNTHESIS****ANSWER ANY EIGHT (8) OF THE NINE (9) QUESTIONS 32-40.**

For each of the questions 32 - 40 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.

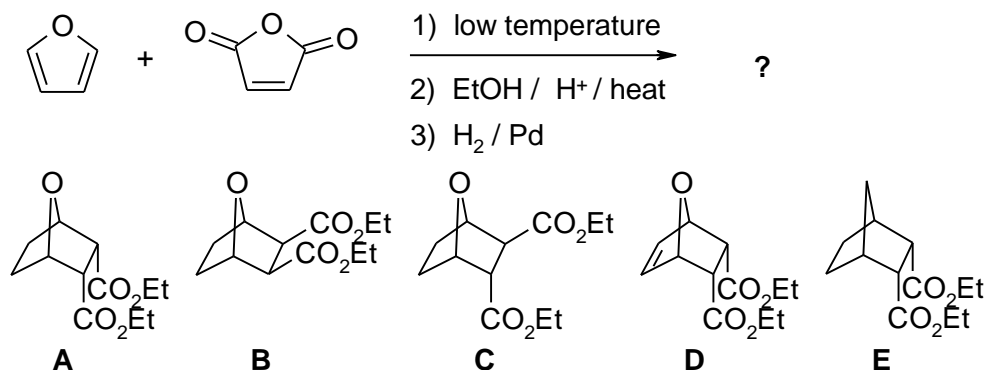
32.



33.



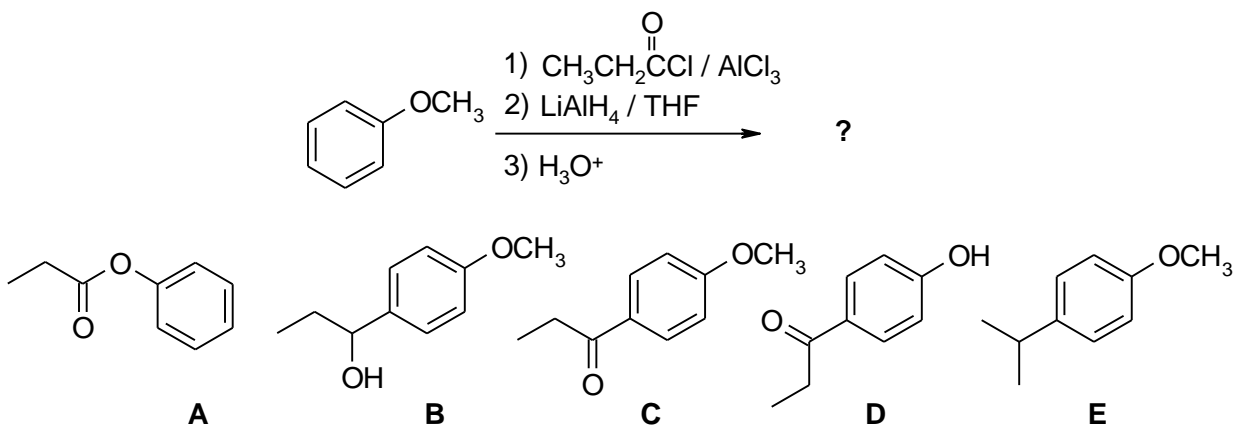
34.



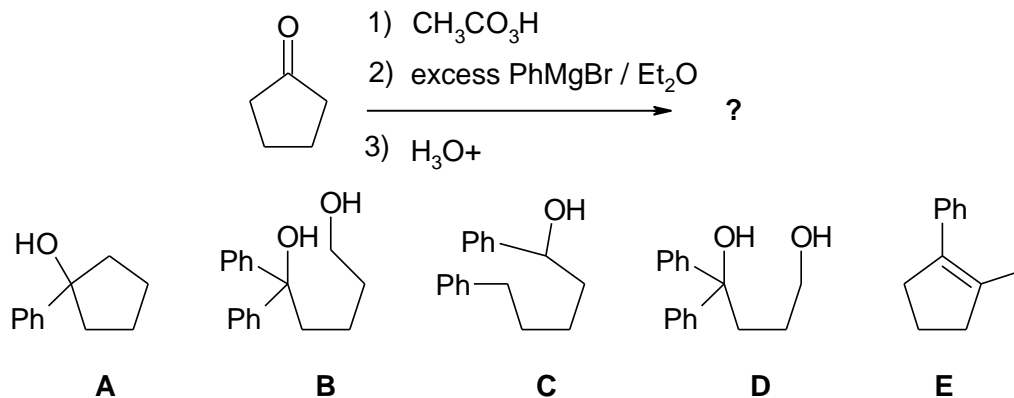
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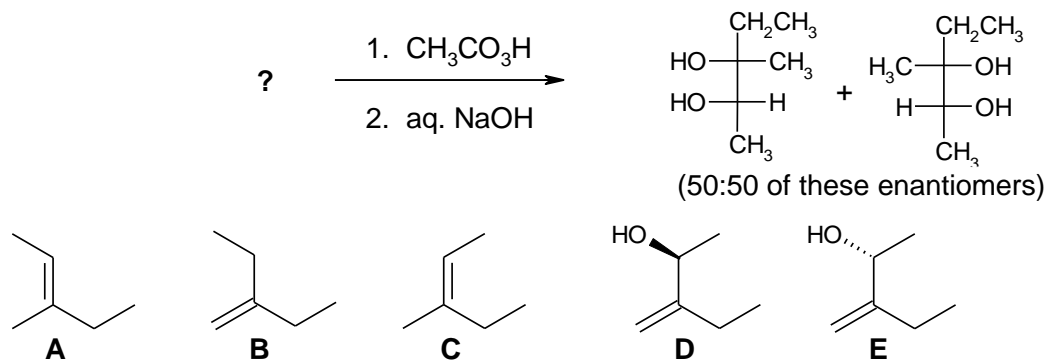
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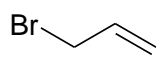
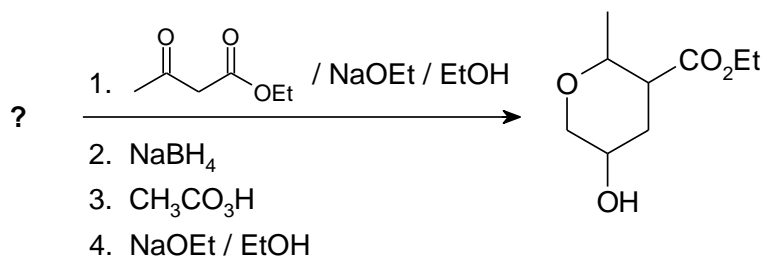
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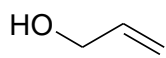
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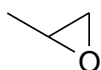
38.



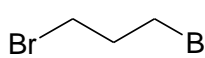
A



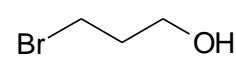
B



C

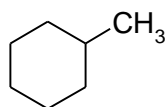
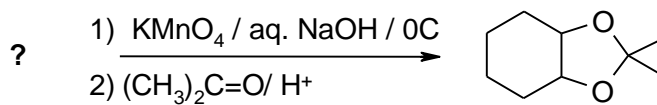


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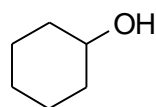


E

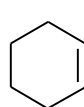
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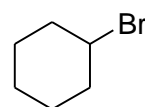
A



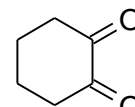
B



C

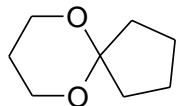
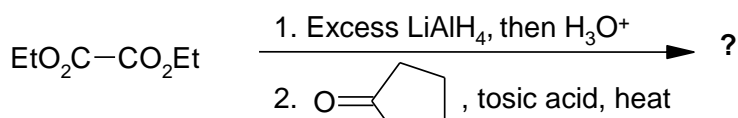


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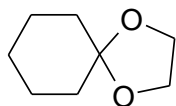


E

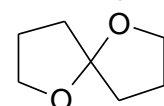
40.



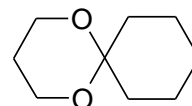
A



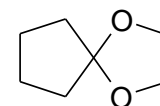
B



C



D

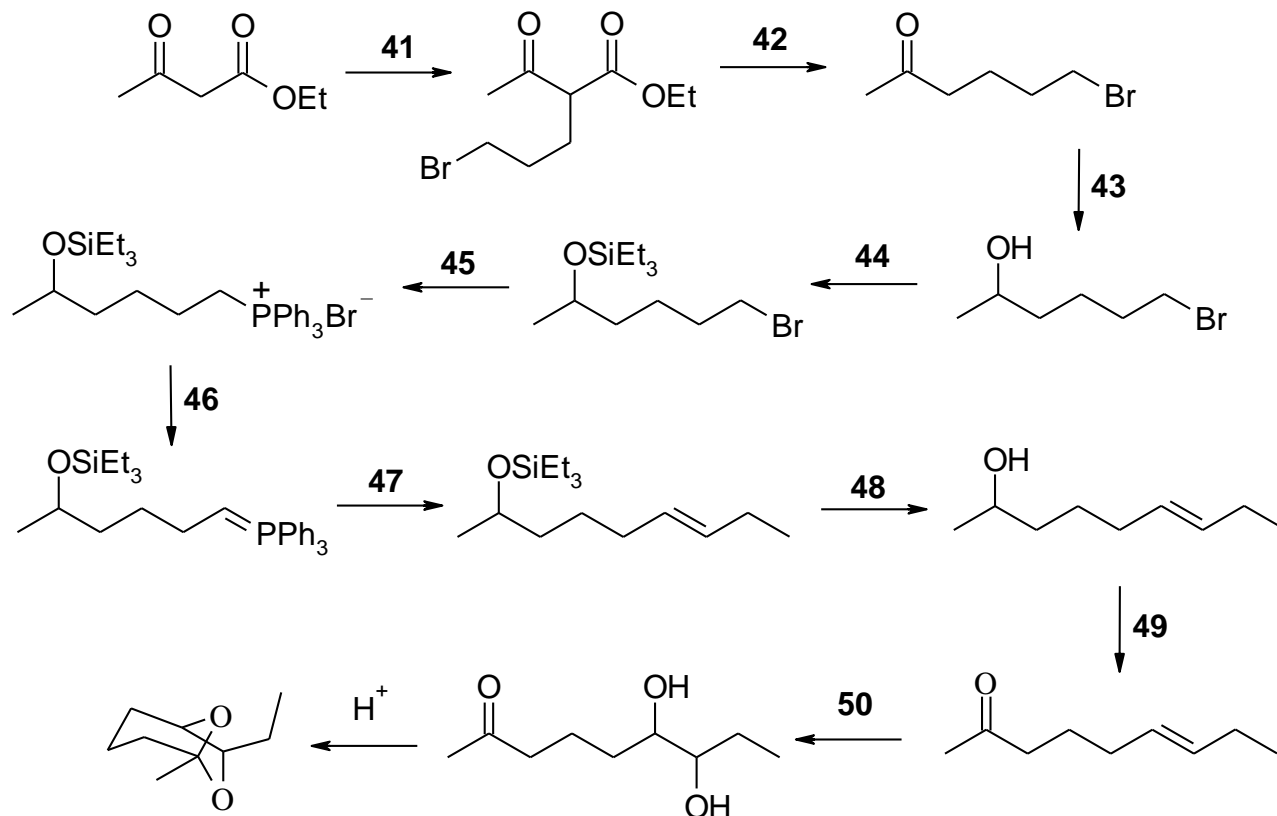


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**10% PART 5: REAGENTS FOR SYNTHESIS****ANSWER ALL OF THE QUESTIONS 41 - 50**

The following reaction scheme shows a possible synthesis of BREVICOMIN, a pheromone of the Western Pine Beetle. From the list of reagents provided in the table below, select the best reagent combination to carry out each of the reactions required at each numbered step.

**BREVICOMIN**

A. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Li} / \text{THF}$	AE. $\text{CH}_2=\text{CHCH}_2\text{Br}$
B. $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$	BC. $\text{H}_3\text{O}^+ / \Delta$
C. $\text{Et}_3\text{SiCl} / \text{Et}_3\text{N}$	BD. $\text{Conc. H}_2\text{SO}_4 / \Delta$
D. $\text{Et}_3\text{SiH} / \text{pyridine}$	BE. $\text{NaOEt then Br(CH}_2)_3\text{Br}$
E. $\text{CH}_3\text{CHO}$	CD. $\text{Et}_3\text{N}$
AB. $\text{CH}_3\text{CH}_2\text{CHO}$	CE. $\text{NaBH}_4 \text{ then } \text{H}_3\text{O}^+$
AC. PDC	DE. $\text{Bu}_4\text{NF then H}_2\text{O}$
AD. $\text{PPh}_3$	ABC. $\text{KMnO}_4 / \text{aq NaOH} / 0^\circ\text{C}$

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7.5% **PART 6: EXPLANATION OF PHENOMENA**

**ANSWER ALL FIVE (5) OF THE QUESTIONS 51 - 55.**

**CHOOSE THE SINGLE EXPLANATION THAT BEST RATIONALISES THE PHENOMENON INDICATED.**

51. When phenyl ethanoate is alkylated with chloroethane /  $\text{AlCl}_3$ , the *para* product is the major product. This is because:

- A. Alkylation usually occurs at the *para* position.
- B. The -Cl group is a weakly deactivating and an *ortho* / *para* director.
- C. The  $-\text{CO}_2\text{CH}_3$  group is an activator and an *ortho* / *para* director.
- D. The -Et group is weakly activating and an *ortho* / *para* director.
- E. The  $-\text{O}_2\text{CCH}_3$  group is an activator and an *ortho* / *para* director.

52. Terminal alkynes react with 9-borabicyclononane (9-BBN) then aq. alkaline hydrogen peroxide to give aldehydes because:

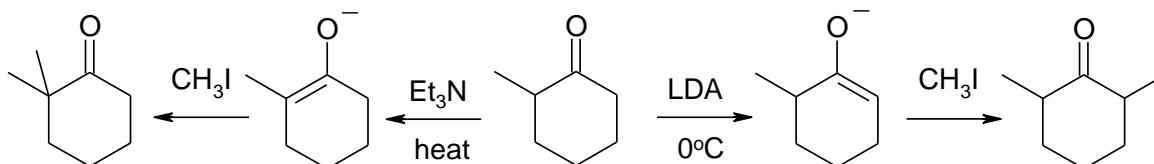
- A. Acid catalysed electrophilic addition of water follows Markovnikov's rule.
- B. Acid catalysed electrophilic addition of water is anti-Markovnikov.
- C. The radical addition is anti-Markovnikov.
- D. Steric and electronic effects cause the boron to the terminal carbon.
- E. Boron attacks the more substituted end of the system due to the cationic character.

53. In general, ketones are more reactive towards nucleophiles than esters because:

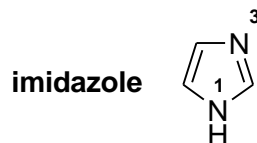
- A. The  $\alpha$ -protons of a ketone are more acidic than those of an ester.
- B. The alkyl group in a ketone is an electron donating group due to hyperconjugation.
- C. Alkoxy (RO-) groups are sterically larger than the related alkyl group.
- D. Alkoxy (RO-) groups are stronger electron donating than alkyl groups via resonance.
- E. Alkoxy (RO-) groups are more electron withdrawing than alkyl groups due to inductive effects.

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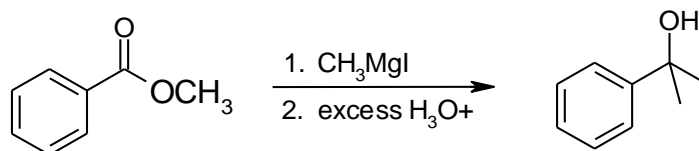
54. When 2-methylcyclohexanone reacts with a base and is then treated with an electrophile such as methyl iodide the product depends on the reaction conditions, see below. At high temperature, the major product is the geminal dimethyl compound. This is because:



- A. Alkyl groups are weak electron donors due to inductive effects and hyperconjugation.  
 B. The enolate formed at high temperature is more stable.  
 C. diisopropyl amide (LDA) is a much stronger base than Et<sub>3</sub>N.  
 D. Lithium diisopropyl amide (LDA) promotes an anti-Markovnikov type addition.  
 E. Lithium diisopropyl amide (LDA) promotes a Markovnikov type addition
55. Imidazole has a pK<sub>a</sub> = 7 with respect to its conjugate acid. Which N is protonated in this conjugate acid and why?



- A. Either because imidazole is an aromatic heterocycle where  $n=1$  in the Huckel rule.  
 B. N1 is protonated because it is  $sp^3$  hybridised.  
 C. N3 is protonated because it is  $sp^2$  hybridised.  
 D. N1 is protonated because the lone pair is part of the aromatic pi system.  
 E. N3 is protonated because the lone pair is not part of the aromatic pi system.

Value**4.5% PART 7: LABORATORY****WRITE YOUR ANSWERS TO BOTH PARTS A and B IN THE BOOKLET PROVIDED.****(2) PART A:**Calculate the % yield of **2-phenylpropan-2-ol** based on the following experimental data:

Methyl benzoate (2.00g) and methyl magnesium iodide (3.32g) in THF (50mL) were stirred at room temperature. After 45 minutes, the mixture was made acidic with cold dilute aqueous acid. The reaction was cooled and allowed to precipitate. The product was collected by vacuum filtration and dried to give crude 2-phenylpropan-2-ol (1.00g).

**(2.5) PART B:**

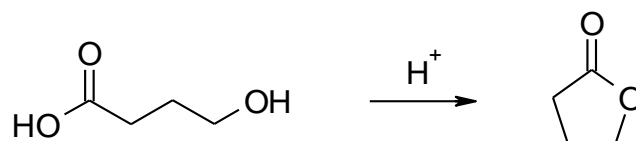
Explain (using point form or a flow chart) how you could use extraction to obtain a sample of pure benzoic acid from a crude reaction mixture containing benzoic acid, bromobenzene, biphenyl and inorganic magnesium salts.

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Value

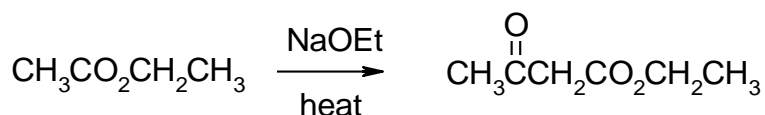
**9% PART 8: MECHANISM****WRITE YOUR ANSWERS IN THE BOOKLET PROVIDED.****NO REAGENTS OTHER THAN THOSE ALREADY SHOWN IN EACH QUESTION ARE REQUIRED.****(4) PART A: Draw the curly arrow mechanism for ONE of the following transformations :**

i.

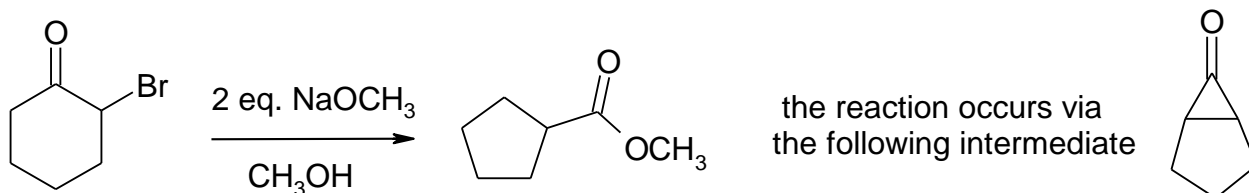


OR

ii.

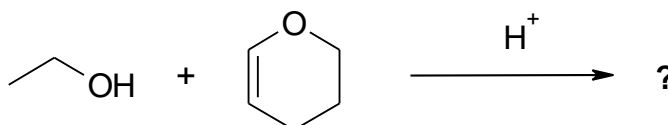
**(5) PART B : Draw the curly arrow mechanism for ONE of the following transformations:**

i. 2-bromocyclohexanone with sodium methoxide to give methyl cyclopentanecarboxylate (shown below). This reaction is also known as the Favorskii reaction.



OR

ii.



CONTINUED --&gt;

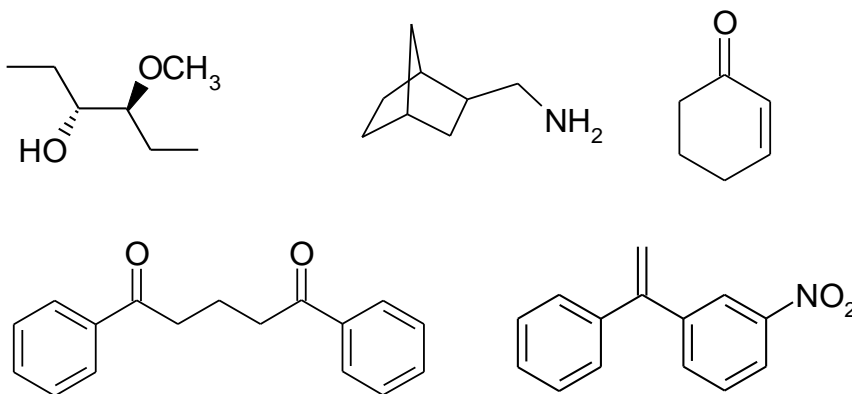
Value

**12% PART 9: TOTAL SYNTHESIS****WRITE YOUR ANSWERS IN THE BOOKLET PROVIDED.**

**Design an efficient synthesis for any THREE (3) of the following target molecules using any of the starting materials and reagents given in the accompanying list.**

**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 **THREE** carbons
- benzene
- cyclopentanol

You can use any solvents or other reagents for the reactions provided that they do not contribute carbon atoms to the target.

CONTINUED --&gt;



Value

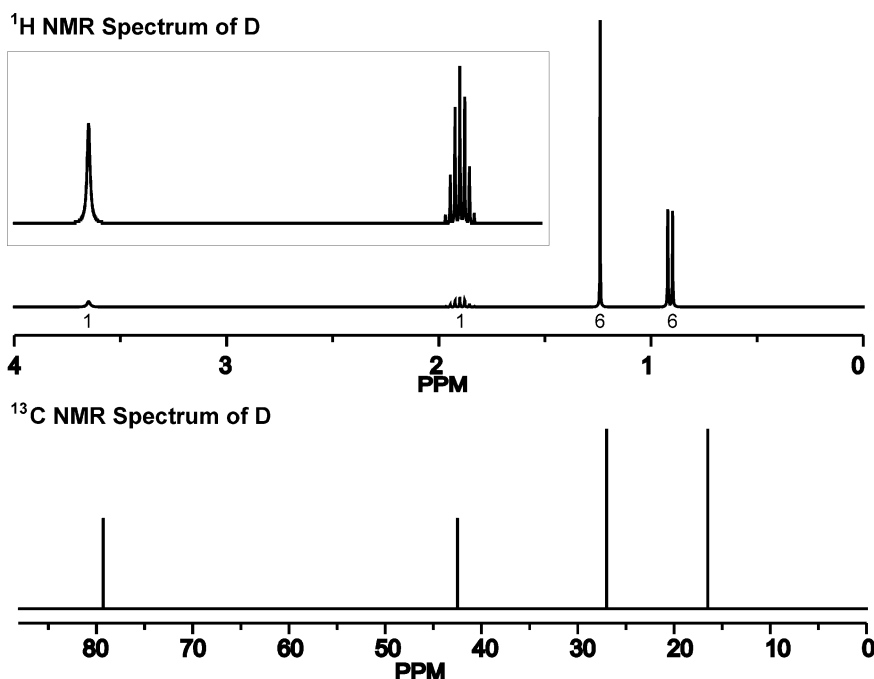
**10% PART 10: STRUCTURE DETERMINATION****WRITE YOUR ANSWERS IN THE BOOKLET PROVIDED**

**A:** mass spectra showed  $M^+ = 88$ , elemental analysis gave 68.13% C and 13.72% H, and IR absorption:  $3500\text{ cm}^{-1}$  (strong broad band). **A** did not react with Jones reagent ( $\text{K}_2\text{Cr}_2\text{O}_7$  in  $\text{H}_2\text{SO}_4$ ); however when **A** was heated with conc. sulfuric acid, hydrocarbon **B** was obtained.

When **B** was subsequently reacted with m-chloroperoxybenzoic acid (MCPBA) it gave compound **C**. Treatment of **C** with methyl magnesium bromide gave **D** after an acid workup. Compound **D** also showed an IR absorption  $3500\text{ cm}^{-1}$  (strong broad band) and gave the  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra shown below.

The treatment of **D** with HBr gave compound **E**, which, upon treatment with potassium tert-butoxide in hot tert-butanol, gave compound **F** as the major compound. When compound **F** was subjected to a reaction with  $\text{O}_3$  followed by  $\text{H}_2\text{O}_2$ , compound **G** and  $\text{CO}_2$  were obtained. Treatment of **G** with methyl magnesium bromide followed by acid workup gave **D** again. However, when **G** was reacted with  $\text{NaBH}_4$  in methanol, compound **H**, a constitutional isomer of **A** was obtained.

Treatment of **G** with m-chloroperoxybenzoic acid (MCPBA) gave **I** as the major compound. Heating **I** with aqueous acid gave ethanoic acid and propan-2-ol.



Identify the compounds **A** to **I** (structures are sufficient).

What is the name of the reaction that converts **G** to **I** ?

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

## PERIODIC TABLE

<b>1</b> 1A																<b>18</b> 8A				
1 <b>H</b> 1.008																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 \*

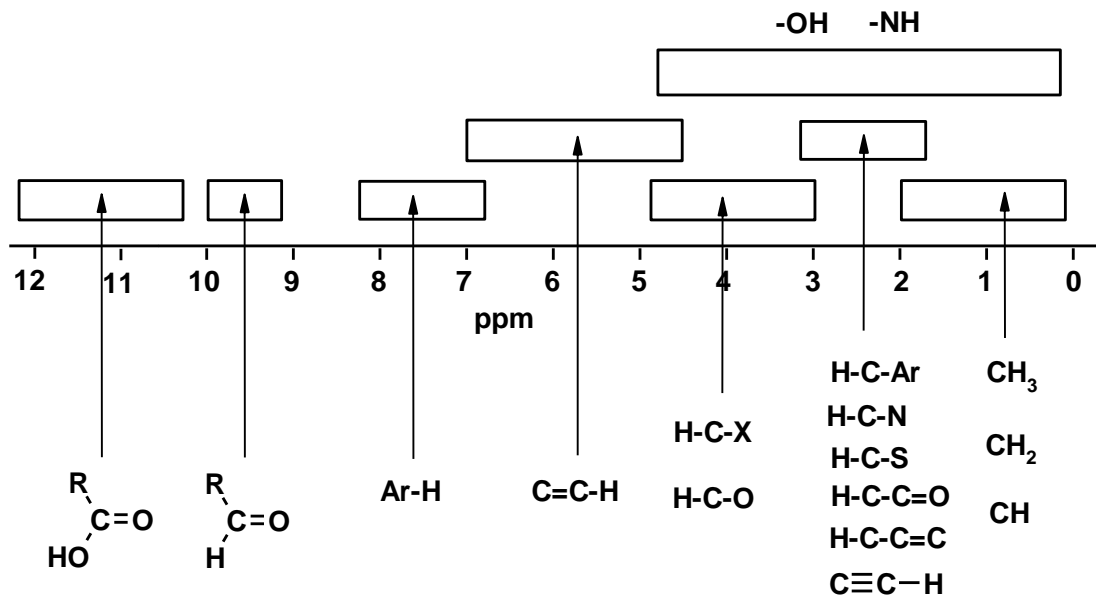
58 <b>Ce</b> 140.1	59 <b>Pr</b> 140.9	60 <b>Nd</b> 144.2	61 <b>Pm</b> (145)	62 <b>Sm</b> 150.4	63 <b>Eu</b> 152.0	64 <b>Gd</b> 157.3	65 <b>Tb</b> 158.9	66 <b>Dy</b> 162.5	67 <b>Ho</b> 164.9	68 <b>Er</b> 167.3	69 <b>Tm</b> 168.9	70 <b>Yb</b> 173.0	71 <b>Lu</b> 175.0
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Actinides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

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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**Schematic diagrams of NMR chemical shift data for  $^1\text{H}$  and  $^{13}\text{C}$  NMR**

**$^1\text{H}$  NMR**

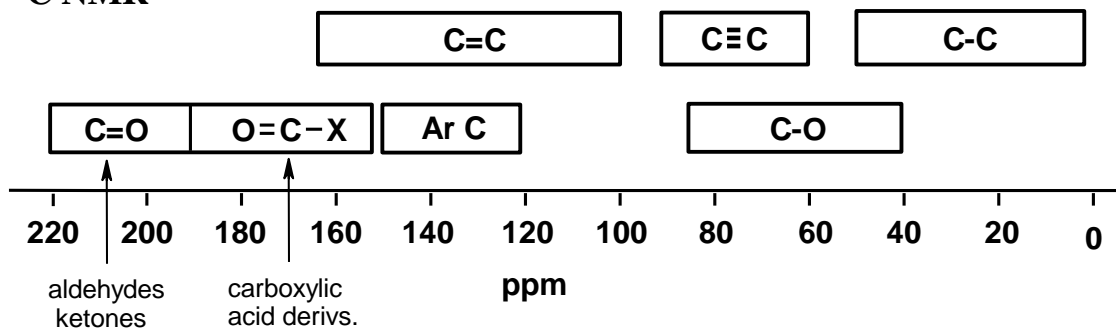


**$^1\text{H}$  NMR CHARACTERISTIC CHEMICAL SHIFTS / ppm**

	methyl CH <sub>3</sub> -	methylene -CH <sub>2</sub> -	methyne CH	other	
$\text{R}-\text{C}-$	0.9	1.4	1.5	-OH	1-5
$\text{R}-\text{C}=\text{C}$	1.6	2.3	2.6	-NH	1-3
$\text{R}-\text{C}(=\text{O})-$	2.1	2.4	2.5	$\text{C}\equiv\text{CH}$	2.5
$\text{R}-\text{N}-$	2.2	2.5	2.9	$\text{C}=\text{C}-\text{H}$	5.5
R-Ar	2.3	2.7	3.0	Ar-H	7.3
R-Br	2.7	3.3	4.1	$\text{R}-\text{C}(=\text{O})-\text{H}$	10
R-Cl	3.1	3.4	4.1	$\text{R}-\text{C}(=\text{O})-\text{OH}$	9-12
R-O-	3.3	3.4	3.7		

CONTINUED -->

**<sup>13</sup>C NMR**



**<sup>13</sup>C NMR CHARACTERISTIC CHEMICAL SHIFTS / ppm**

$\text{—CH}_3$ 0-30	$\text{>CH}_2$ 10-50	$\text{—}\overset{\text{H}}{\underset{\text{H}}{\text{C}}}\text{—}$ 25-60	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—O—}$ 155-180
$\text{—C}\equiv\text{C—}$ 65-90	$\text{—}\overset{\text{H}}{\underset{\text{H}}{\text{C}}}\text{—Br}$ 10-25	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—OH}$ 160-185	
$\text{>C=C<}$ 80-145	$\text{—}\overset{\text{H}}{\underset{\text{H}}{\text{C}}}\text{—Cl}$ 15-30	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—H}$ 190-210	
 110-170	$\text{—}\overset{\text{H}}{\underset{\text{H}}{\text{C}}}\text{—OH}$ 45-75	$\text{—}\overset{\text{O}}{\parallel}{\text{C}}\text{—}$ 190-220	

CONTINUED -->

**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

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

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