
OpenCourseWare (2023)

CHEMISTRY II

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SOLUTIONS OF EVALUATION TEST 1



1. (3 points) Mark the correct answer, there is only one correct in each question. (Correct answers mark as +1, incorrect ones mark as - 0.2, and non-answered questions mark as 0. The resulting mark will not be smaller than 0 in any case).

A	Given the following standard reduction potentials:										
	<table border="1"> <thead> <tr> <th><i>Redox Pair</i></th> <th>E° (V)</th> </tr> </thead> <tbody> <tr> <td>Ag⁺/Ag</td> <td>+0.80</td> </tr> <tr> <td>Cl₂/Cl⁻</td> <td>+1.36</td> </tr> <tr> <td>NO₃⁻/NO</td> <td>+0.96</td> </tr> <tr> <td>Na⁺/Na</td> <td>-2.71</td> </tr> </tbody> </table>	<i>Redox Pair</i>	E° (V)	Ag ⁺ /Ag	+0.80	Cl ₂ /Cl ⁻	+1.36	NO ₃ ⁻ /NO	+0.96	Na ⁺ /Na	-2.71
	<i>Redox Pair</i>	E° (V)									
	Ag ⁺ /Ag	+0.80									
	Cl ₂ /Cl ⁻	+1.36									
	NO ₃ ⁻ /NO	+0.96									
Na ⁺ /Na	-2.71										
Mark the correct statement:											
Cl ⁻ is a stronger reducing agent than NO.											
NO ₃ ⁻ is a strong reducing agent.											
X	Ag metal can be oxidized spontaneously in the presence of Cl₂.										
	Na ⁺ and Ag ⁺ will be always reduced spontaneously to Na and Ag, respectively, in the presence of a reducing agent.										

B	Regarding Crevice corrosion, select the correct answer:
	It takes place when two metals are electrically coupled.
X	It occurs in the region of the metal that has the lower oxygen concentration.
	It occurs when a force is applied to the metal.
	It is favored in uniform surfaces.

C	Regarding reactivity of substituted aromatic compounds, select the correct statement:
	Nitro group accepts electron density from the ring by induction.
	Hydroxyl groups can accept electron density by resonance.
	Methyl group is an electron donor group by resonance.
X	Nitro group is an electron withdrawing group by resonance.

D	Select the correct statement:
X	p-Hydroxybenzaldehyde is less acidic than p-nitrophenol.
	Haloalkanes have higher boiling points than alcohols.
	Acidity of alcohols is lower than that of the alkanes and haloalkanes.
	In carbonyl compounds, oxygen atom is electrophilic and slightly basic.

E	An enzyme that follows Michaelis-Menten kinetics has a catalytic constant of 900 s^{-1} and K_m for the substrate of $40 \text{ }\mu\text{M}$. When substrate concentration is $50 \text{ }\mu\text{M}$, the reaction velocity, V_0 , is $20 \text{ }\mu\text{M}\cdot\text{s}^{-1}$. Determine the V_{max} in presence of an inhibitor if a competitive inhibition is followed.
	$18 \text{ }\mu\text{M}\cdot\text{s}^{-1}$
X	$36 \text{ }\mu\text{M}\cdot\text{s}^{-1}$
	$72 \text{ }\mu\text{M}\cdot\text{s}^{-1}$
	$45 \text{ }\mu\text{M}\cdot\text{s}^{-1}$

F	Select the wrong statement:
X	The anomeric carbon, which corresponds to the most reduced carbon of a cyclized monosaccharide, is chiral.
	Presence of double bonds in fatty acids produces bends in the hydrocarbon chain which avoid close packing and van der Waals interactions and consequently melting point is lower than that in saturated fatty acids.
	The information contained in the sequence of one strand of DNA is conserved in the sequence of the other strand.
	The peptide bonds link amino acids in proteins and they are rigid and planar.

2. (1.5 points) Magnesium metal (6.00 g) is electroplated from molten magnesium chloride using a current of 7.50 A during 2 h. Determine the volume (in L) of chlorine gas at $25 \text{ }^\circ\text{C}$ and 1.00 atm that is produced at the anode.

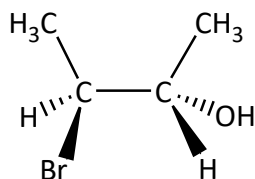
Data: Atomic mass: Mg = 24.3; F = 96500 C/mol e^- .

SOLUTION

$$n(\text{Cl}_2) = 7.5 \text{ A} \cdot 2 \cdot 60 \cdot 60 \text{ s} / 2 \cdot 96500 = 0.2798 \text{ mol}$$

$$V(\text{Cl}_2) = 0.2798 * 0.082 * 298 / 1 = 6.84 \text{ L}$$

3. (1.5 points) In the enclosed figure you may find the 3D structural formula of 2-bromo-3-butanol.



a) (0.5 p) Find how many quiral centers exist and determine their configuration (*R* or *S*) in the current figure.

b) (0.6 p) Draw the Newman projection along the C2-C3 axis (C2 in front) and draw a scheme of the variation of the potential energy as a function of rotation angle in 60° steps assuming that the main substituents (–CH₃, –OH, and –Br) have the same size. How many maxima appear in a 360° rotation?

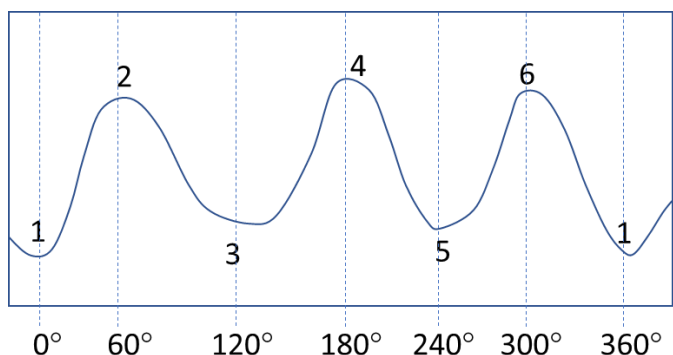
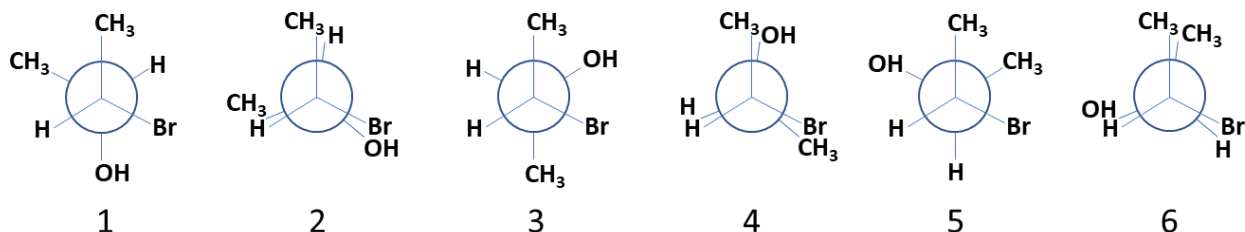
c) (0.4 p) Haloalkanes contain an electrophilic carbon atom, which may react with nucleophiles. Identify each of the following statements for nucleophilic substitution reactions that occur through the S_N1 or S_N2 mechanism:

	S _N 1	S _N 2
1. Primary and most secondary haloalkanes react with nucleophiles through this mechanism.		
2. It is a stereospecific reaction and proceeds by posterior displacement, thus, producing the inversion of the configuration in the reaction center.		
3. Nucleophilicity increases with negative charge, and in polar aprotic solvents.		
4. Secondary haloalkanes undergo a slow substitution reaction while tertiary ones undergo rapid substitution in polar media.		
5. The slowest step, or speed determining factor, in this substitution, is the dissociation of the C-X bond to form an intermediate carbocation.		
6. The transition state implies a planar trigonal sp ² hybridized carbon center.		
7. When the solvent acts as a nucleophile, the process is called solvolysis.		
8. Substitution is favored by unhindered substrates and small, less basic nucleophiles.		

SOLUTION

a) Two quiral centers, C2 and C3. Both are in S configuration.

b) Newman projections:



Energy:
 $4 > 2 = 6 > 3 = 5 > 1$

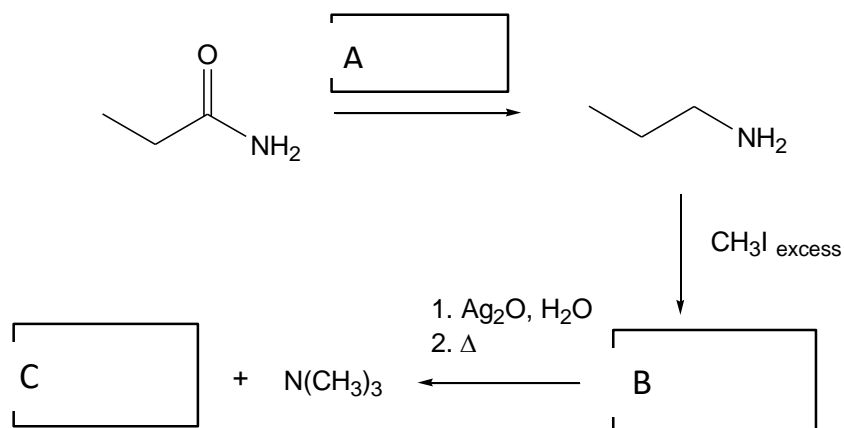
There are three maxima.

c)

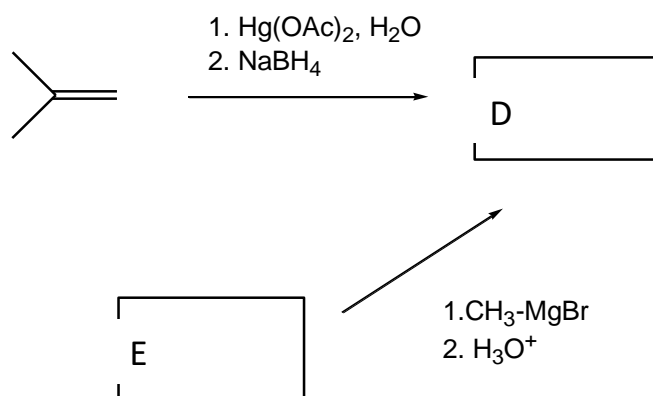
	S_N1	S_N2
1. Primary and most secondary haloalkanes react with nucleophiles through this mechanism.		X
2. It is a stereospecific reaction and proceeds by posterior displacement, thus, producing the inversion of the configuration in the reaction center.		X
3. Nucleophilicity increases with negative charge, and in polar aprotic solvents.		X
4. Secondary haloalkanes undergo a slow substitution reaction while tertiary ones undergo rapid substitution in polar media.	X	
5. The slowest step, or speed determining factor, in this substitution, is the dissociation of the C-X bond to form an intermediate carbocation.	X	
6. The transition state implies a planar trigonal sp^2 hybridized carbon center.		X
7. When the solvent acts as a nucleophile, the process is called solvolysis.	X	
8. Substitution is favored by unhindered substrates and small, less basic nucleophiles.	X	

4. (2.5 points) Complete the following schemes:

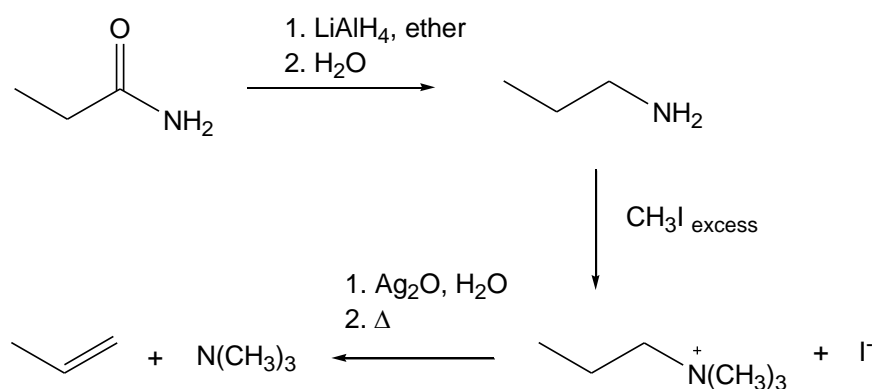
Scheme 1 (1.5 p)

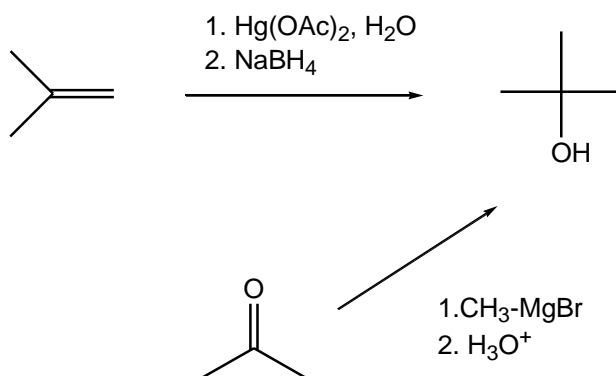


Scheme 2 (1 p)



SOLUTION





5. (1.5 points) A compound with formula $\text{C}_8\text{H}_{10}\text{O}$ exhibits the following ^1H NMR spectrum: $\delta = 1.50$ (doublet, 3 H), 1.90 (broad singlet, 1 H), 4.75 (quartet, 1 H), 7.20-7.35 (multiplet, 5 H) ppm. Moreover, this compound shows an infrared absorption peak, among others, at 3547 cm^{-1} .

a) (1 p) Deduce its structure.

b) (0.5 p) Justify how many signals you would expect this compound to have in its ^{13}C NMR spectrum.

SOLUTION

a) *Degree of unsaturation* = $(8 + 1) - \frac{(9+1)}{2} = 4$

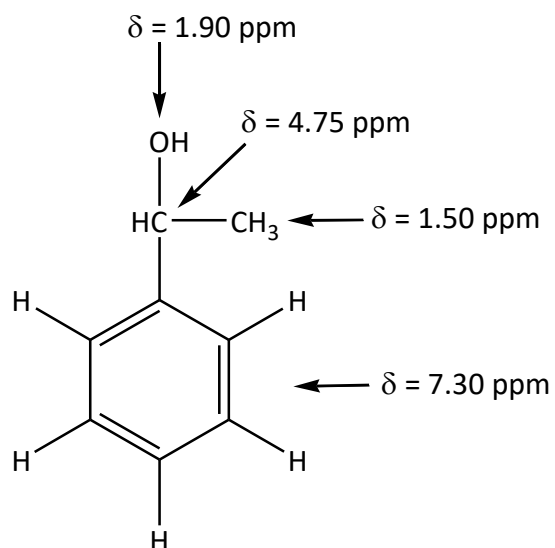
IR spectrum gives the information that there is an alcohol in the structure.

The signals that can be observed in the NMR spectrum are:

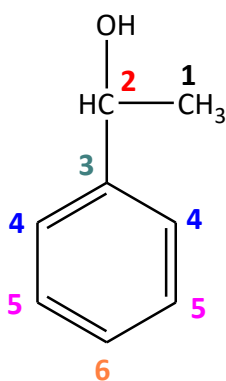
- A doublet that integrates three protons centered at approximately 1.5 ppm.
- A singlet with an integral of 1 H situated at a value of 1.90 ppm.
- A quartet that also integrates a proton centered at 4.75 ppm value.
- A multiplet with a 5 protons integral located in the range 7.20-7.35 ppm.

From a first observation of the proton NMR spectrum data and considering the degree of unsaturation, we can deduce that it is a monosubstituted aromatic ring (multiplet at $\delta = 7.20\text{-}7.35$ ppm.). The signal present at higher field is a doublet that integrates 3 H (a group $-\text{CH}_3$), so much it will be coupled with a proton that it will consequently unfold into a quartet ($\delta = 4.75$ ppm), which to be at such low field will suffer the unprotection effect of the oxygen from the OH group and the benzene ring. Finally, the singlet present at 1.90 ppm will correspond to the proton of the OH group.

Therefore, the proposed structure would be the following:



b) There will be six different peaks in the ^{13}C spectrum:



ANNEX

Chemical Shifts in ^1H NMR

Type of hydrogen		Chemical shift (δ)
Reference	$\text{Si}(\text{CH}_3)_4$	0
Alkyl (primary)	$-\text{CH}_3$	0.7–1.3
Alkyl (secondary)	$-\text{CH}_2-$	1.2–1.6
Alkyl (tertiary)	$\begin{array}{c} \\ -\text{CH}- \\ \end{array}$	1.4–1.8
Allylic	$\begin{array}{c} \text{H} \\ \\ \text{C}=\text{C}-\text{C}- \\ \end{array}$	1.6–2.2
Methyl ketone	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{CH}_3 \end{array}$	2.0–2.4
Aromatic methyl	$\text{Ar}-\text{CH}_3$	2.4–2.7
Alkynyl	$-\text{C} \equiv \text{C}-\text{H}$	2.5–3.0
Alkyl halide	$\begin{array}{c} \text{H} \\ \\ -\text{C}-\text{Hal} \\ \end{array}$	2.5–4.0
Alcohol	$\begin{array}{c} \\ -\text{C}-\text{O}-\text{H} \\ \end{array}$	2.5–5.0
Alcohol, ether	$\begin{array}{c} \text{H} \\ \\ -\text{C}-\text{O}- \\ \end{array}$	3.3–4.5
Vinylic	$\begin{array}{c} \text{H} \\ \\ \text{C}=\text{C} \\ \end{array}$	4.5–6.5
Aryl	$\text{Ar}-\text{H}$	6.5–8.0
Aldehyde	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{H} \end{array}$	9.7–10.0
Carboxylic acid	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{O}-\text{H} \end{array}$	11.0–12.0

Characteristic IR bands of some common functional groups:

Functional Group		Absorption (cm^{-1})	Intensity
Alkane	C-H	2850–2960	Medium
Alkene	=C-H	3020–3100	Medium
	C=C	1640–1680	Medium
Alkyne	$\equiv\text{C-H}$	3300	Strong
	$\text{C}\equiv\text{C}$	2100–2260	Medium
Alkyl halide	C-Cl	600–800	Strong
	C-Br	500–600	Strong
Alcohol	O-H	3400–3650	Strong, broad
	C-O	1050–1150	Strong
Arene	C-H	3030	Weak
Aromatic ring		1660–2000	Weak
		1450–1600	Medium
Amine	N-H	3300–3500	Medium
	C-N	1030–1230	Medium
Carbonyl compound	$\text{C}=\text{O}$	1670–1780	Strong
	Aldehyde	1730	Strong
	Ketone	1715	Strong
	Ester	1735	Strong
	Amide	1690	Strong
	Carboxylic acid	1710	Strong

IMAGE CREDITS

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