الإجابة النموذجية لامتحان الكيمياء العضوية الطيفية

ك٣١٧

(ورقة امتحانية كاملة)

الفرقة : الثالثة

الشعبة : الكيمياء و الحيوان ، الكيمياء و الحشرات، الكيمياء و الجيولوجيا، الكيمياء و النبات، الكيمياء التطبيقية و الكيمياء الاشعاعية

التاريخ : السبت ١٤ / ١ / ٢٠١٧

الممتحن : د/ محمد عبد الرحمن موسى ابو ريا

قسم : الكيمياء

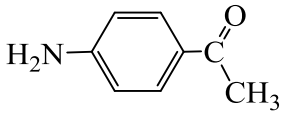
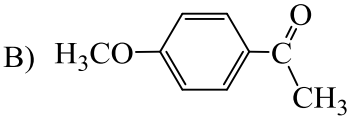
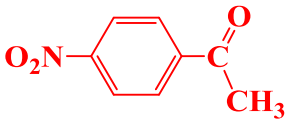
كلية : العلوم

I- Choose the correct answer:

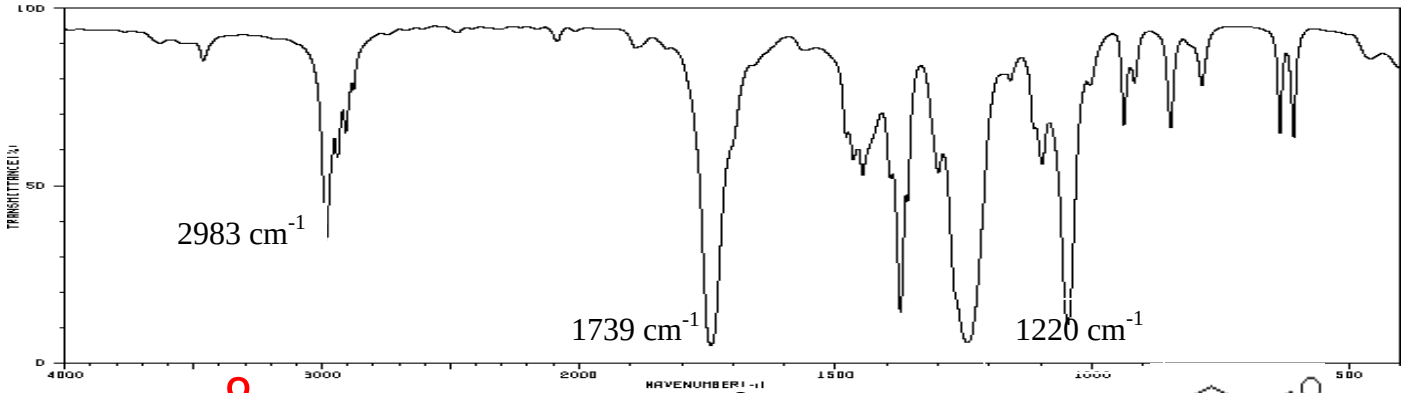
1) Which compound would be expected to show intense IR absorption at 3300 cm^{-1}?

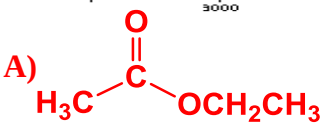
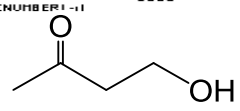
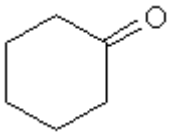
A) but-1-ene B) $H_3C-C\equiv C-CH_3$ **C)** $H_3C-C\equiv C-H$

2) Which of the following has a C=O stretch that occurs at the highest stretching frequency?

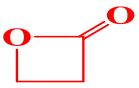
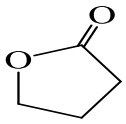
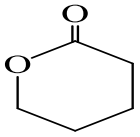
A)  B)  **C)** 

٣) Which of the following compounds match with the following IR spectrum:

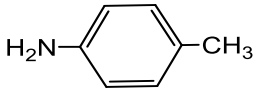


A)  B)  C) 

4) Which compound would be expected to show highest stretching frequency of carbonyl group?

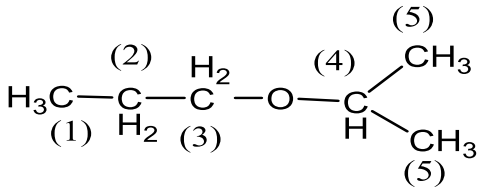
A)  B)  C) 

5) How many signals you would expect the following molecule to have in its ^1H NMR spectra:



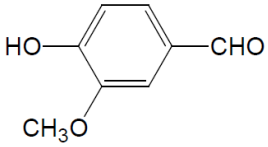
A) 3 **B) 4** C) 5

6) Which proton(s) of the following compound would appear as a triplet in the ^1H NMR spectrum?



A) protons on carbon 3 & 1 B) protons on carbon 3 & 5 C) protons on carbon 1

7)How many ^1H NMR signals does vanillin give?



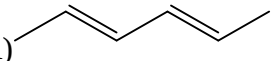
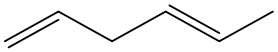
vanillin

A) 4 B) 5 **C) 6**

8) A signal has been reported at chemical shift equal 2 ppm in an NMR spectrometer operating at 400 MHz, the hertz downfield from TMS would be

A) 400 Hz B) 200 Hz **C) 800 Hz**

٩) Which of the following compounds exhibits the highest wave length in its UV spectrum.

A)  **B)**  C) 

١٠) Which compound gives M and M^{+2} peaks in the mass spectrum ؟

A) $C_4H_{10}O$ B) $C_4H_{11}N$. **C) C_4H_9Cl.**

11) The mass spectrometry detects the……molecules

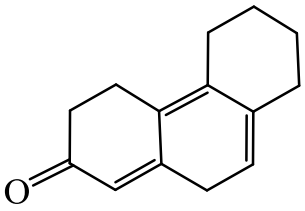
A) radical cation B) cation **C) A&B**

12) An odd molecular ion peak usually indicates the presence of an ……. number of nitrogen atoms in the molecule.

A) even **B) odd** C) even and odd

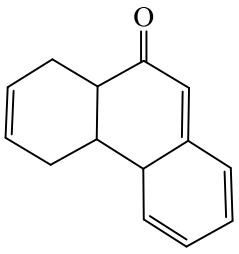
II- *a)* Calculate the λ_{max} for each of the following compounds:

α,β-unsaturate ketones	215
Homoannular diene	39
Extended double bond	2 x 30
Exocyclic double bond	4 x 5
Ring residue and alkyl substituted	
β-Substituent	1 x 12
γ-Substitutent	1 x 18
δ- Substitutent	1 x 18
higher than δ	2 x 18
λmax (calc.)	418 nm



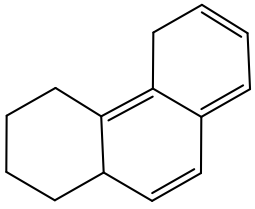
(I)

α,β-unsaturate ketones	215
Homoannular diene	39
Extended double bond	2 x 30
Exocyclic double bond	1 x 5
Ring residue and alkyl substituted	
β-Substituent	1 x 12
higher than δ	1 x 18
λmax (calc.)	349 nm



(II)

Homo annular diene	253 nm
Extended double bond	2 x 30 nm
Exocyclic double bond	3 x 5 nm
Ring residue and alkyl substituted	5 x 5 nm
λmax (calc.)	353 nm



(III)

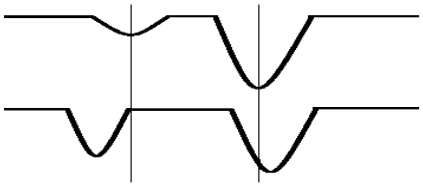
b) **Define each of the following:**

i- Base beak: It is the tallest peak in the mass spectrum corresponding to the most abundant ion in the spectrum 100% abundance.

ii- Overtone Bands: Overtone bands in an infrared spectrum are analogous and are multiples of the fundamental absorption frequency (2 υ′)

iii- Bathochromic shift: shift to longer wave length λ, also called red shift.

iv- Fermi Resonance: The Fermi resonance effect usually leads to two bands appearing close together when only one is expected. When an overtone or a combination band has the same frequency as, or a similar frequency to, a fundamental, two bands appear, split either side of the expected value and are of about equal intensity.



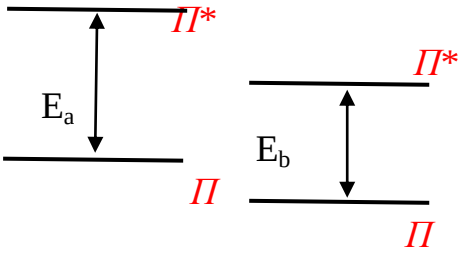
v- parent peak: It is a peak corresponding to the radical cation with the highest molecule weight. It is the heaviest peak in the spectrum.

vi- Auxochromes: It is a functional group of atoms with nonbonded electrons when attached to a chromophore, alters both the wavelength and intensity of absorption. If these groups are in direct conjugation with the pi-system of the chromophore, they may increase the wavelength such as hydroxyl group (-OH), the amino group (-NH_2).

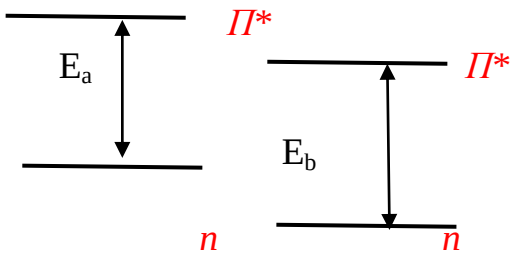
III-

a) Explain the effect of polar solvents on *n* → *Π and *Π* → *Π**** **transition.**

Answer



In polar solvent



In polar solvent

The *Π** orbitals are more stabilized by polar solvents by forming hydrogen bond so the bond shifted to longer wave length ($E_a > E_b$) Bathochromic shift.

The *n* orbitals for unshared electrons are more stabilized by polar solvents the bond shifted to shorter wave length ($E_b > E_a$) Hypsochromic shift.

b) How can you distinguish between the following pairs of compounds (using only IR or ^{1}H NMR spectra)?

i- 1-Bromopropane and 2-bromopropane.

Answer

By using ^{1}H NMR spectra 1-bromopropane gives three sets of protons (triplet, 3H for $-CH_3$ group, multiplet, 2H for $-CH_2-$ group and triplet, 2H for terminal $-CH_2-$) 2-bromopropane gives two sets of protons (douplet, 6H for two $-CH_3$ groups and septet, 1 H for -CH- group)

ii- Propionic acid & 2-propanol.

Answer

By using ^{1}H NMR spectra propanoic gives three sets of protons (triplet, 3H for $-CH_3$ group, quartet, 2H for $-CH_2-$ group and singlet, 1H for acidic proton higher than $\delta = 10$). 1-propanol gives four sets of protons (triplet, 3H for $-CH_3$ group, multiplet, 2H for $-CH_2-$ group, triplet, 2H for $-CH_2-$ and singlet for 1H of hydroxyl group).
Or by using IR spectra propionic acid gives broad band from 2500 to 3400 cm^{-1} for OH of acid and gives also intense beak at 1720 cm^{-1} for carbonyl group.

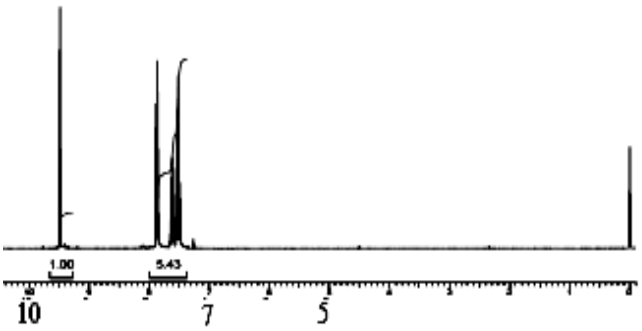
iii- Toluene & methyl cyclohexane.

Answer

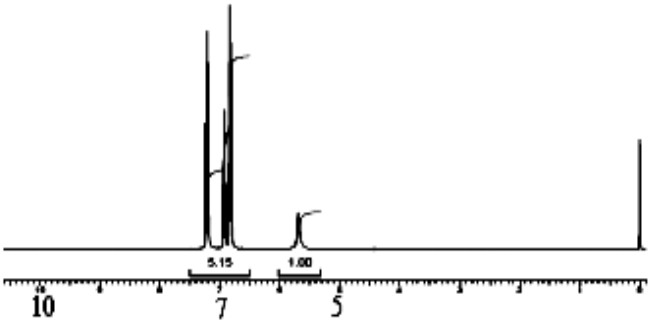
By using ^{1}H NMR spectra toluene gives a characteristic beak between chemical shift 7-8 ppm for =CH of aromatic group.

c) The two spectra below are of phenol and benzaldehyde. Assign them. (3 Marks)

benzaldehyde



phenol



The first figure shows a characteristic beak at chemical shift 9.5 ppm for -CH of aldehydic carbon atom.

IV-

a- **Identify the unknown compound that shows the following spectral data and its elemental analysis data is: C, 81.04; H, 8.16.**

Answer

First we should indicate the molecular weight from the **mass spectroscopy** and elemental analysis as following :

O% = 100- (81.04 + 8.16) = 10.8 %

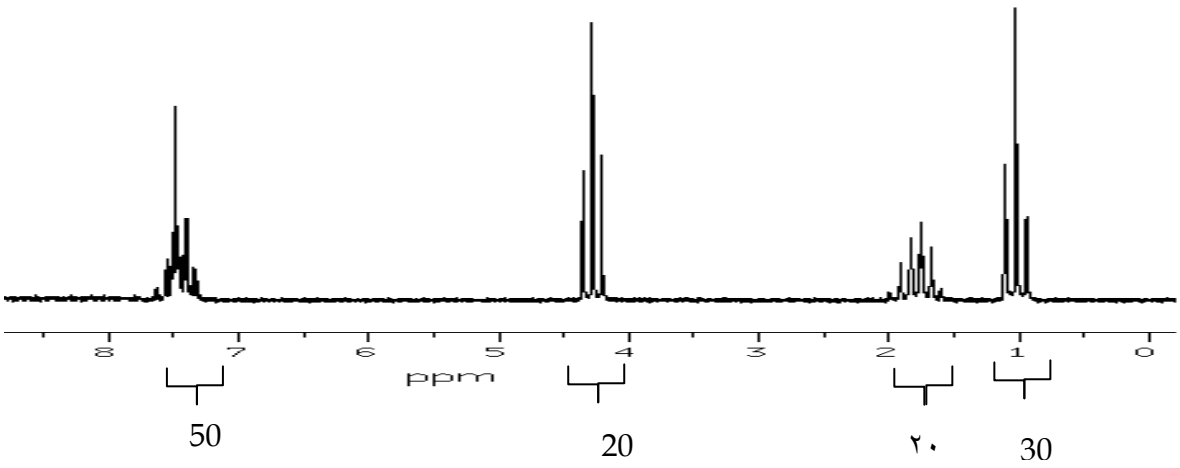
C	H	O
81.04 / 12	8.16/1	10.8 /16
6.75/0.675	8.16/0.675	0.63/0.675
10	12	1

The Empirical formula is $C_{10}H_{12}O$ with Formula weight = 148 is equal to molecular formula shown in **Mass Spectra** so the empirical formula is the molecular formula.

U.N (I.H.D)= (2x10+2-12)/2 = 5

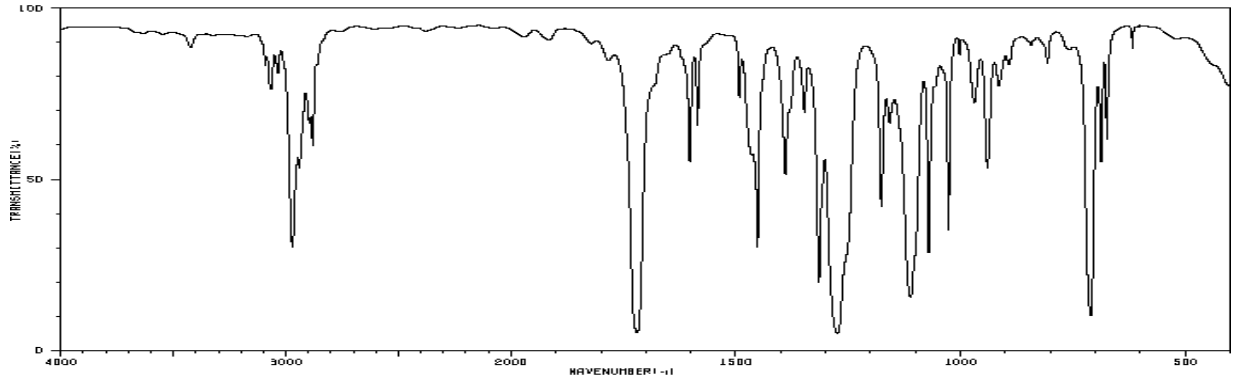
This means presence of aromatic ring and double bond

From ^{1}HNMR spectra



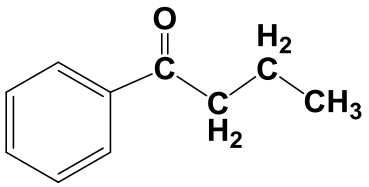
	a	b	c	d
δ	1.1	1.8	4.2	7.4
Multiplicity	triplet	multiplet	quartet	multiplet
Ratio	30	20	20	50
Number of protons	3 H	2 H	2 H	5H
Groups	(-CH_3)	(-CH_2)	(-CH_2)	Aromatic ring

From IR spectra it shows that:



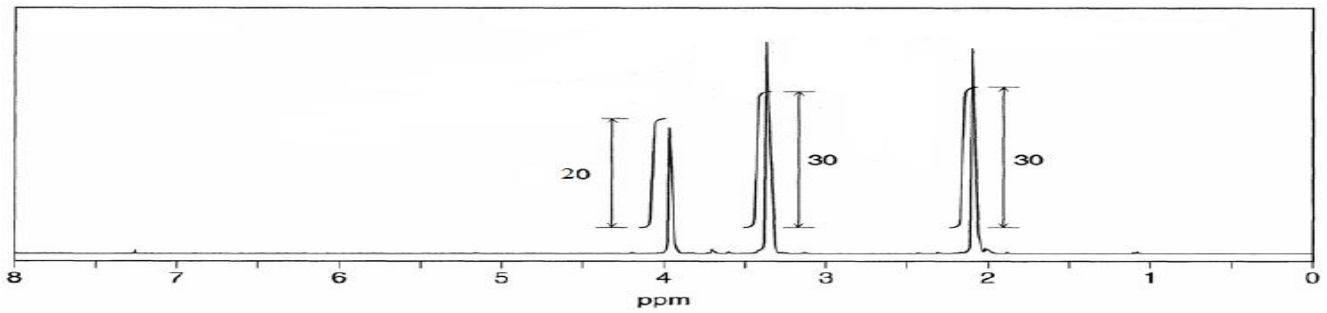
band at ʊ' 3010 cm^{-1} for =CH, band at ʊ' at 2950 cm^{-1} for -CH, band at ʊ' at 1720cm^{-1} for C=O and band at ʊ' at 1600cm^{-1} for C=C.

From the above data the unknown compound is:



b- An organic compound C with molecular formula $C_4H_8O_2$ gives a strong IR peak at 1720 cm^{-1}.

The ^1H NMR spectrum is shown below. What is the structure of C?



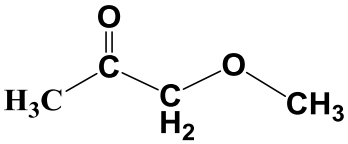
Answer

From IR spectra it shows presence of carbonyl group.

From 1HNMR spectra

	a	b	c
δ	1.1	1.8	4.2
Multiplicity	singlet	singlet	singlet
Ratio	30	30	20
Number of protons	3 H	3 H	2 H
Groups	($-CH_3$)	($-CH_3$)	($-CH_2$)

The compound C is:



With my best wishes,

MOHAMED ABO-RIYA