IR questions

Q1/ (Researchers used a combustion method to analyze a compound used as an antiknock additive in gasoline. A 9.394-mg sample of the compound yielded 31.154 mg of carbon dioxide and 7.977 mg of water in the combustion.

(a) Calculate the percentage composition of the compound.

(b) Determine its empirical formula.

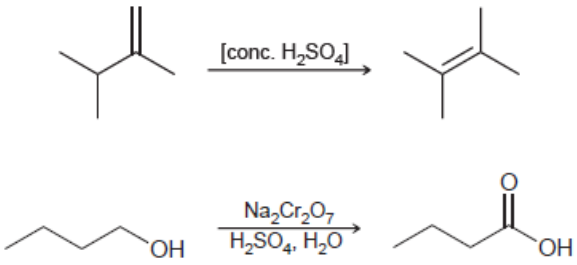
Q2/ An important amino acid has the percentage composition C 32.00%, H 6.71%, and N 18.66%. Calculate the empirical formula of this substance.

Q3/ A substance has the molecular formula C4H9N. Is there any likelihood that this material contains a triple bond? Explain your reasoning.

a. An oxygen-containing compound shows an absorption band at ~1700 cm^{-1} and no absorption bands at ~3300 cm^{-1}, ~2700 cm^{-1}, or ~1100 cm^{-1}. What class of compound is it?
b. A nitrogen-containing compound shows no absorption band at ~3400 cm^{-1} and no absorption bands between 1700 cm^{-1} and 1600 cm^{-1}. What class of compound is it?

Q4/

Q5/ Identify how IR spectroscopy might be used to monitor the progress of the following reactions?



Q6/

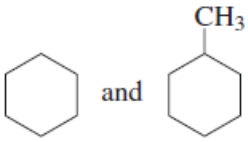
For each of the following pairs of compounds, give one absorption band that could be used to distinguish between them:

a. $CH_3CH_2CH_2CH_3$ and $CH_3CH_2OCH_3$

b. $CH_3CH_2\overset{\overset{O}{\|}}{C}OCH_3$ and $CH_3CH_2\overset{\overset{O}{\|}}{C}OH$

c. $CH_3CH_2\overset{\overset{O}{\|}}{C}OH$ and $CH_3CH_2CH_2OH$

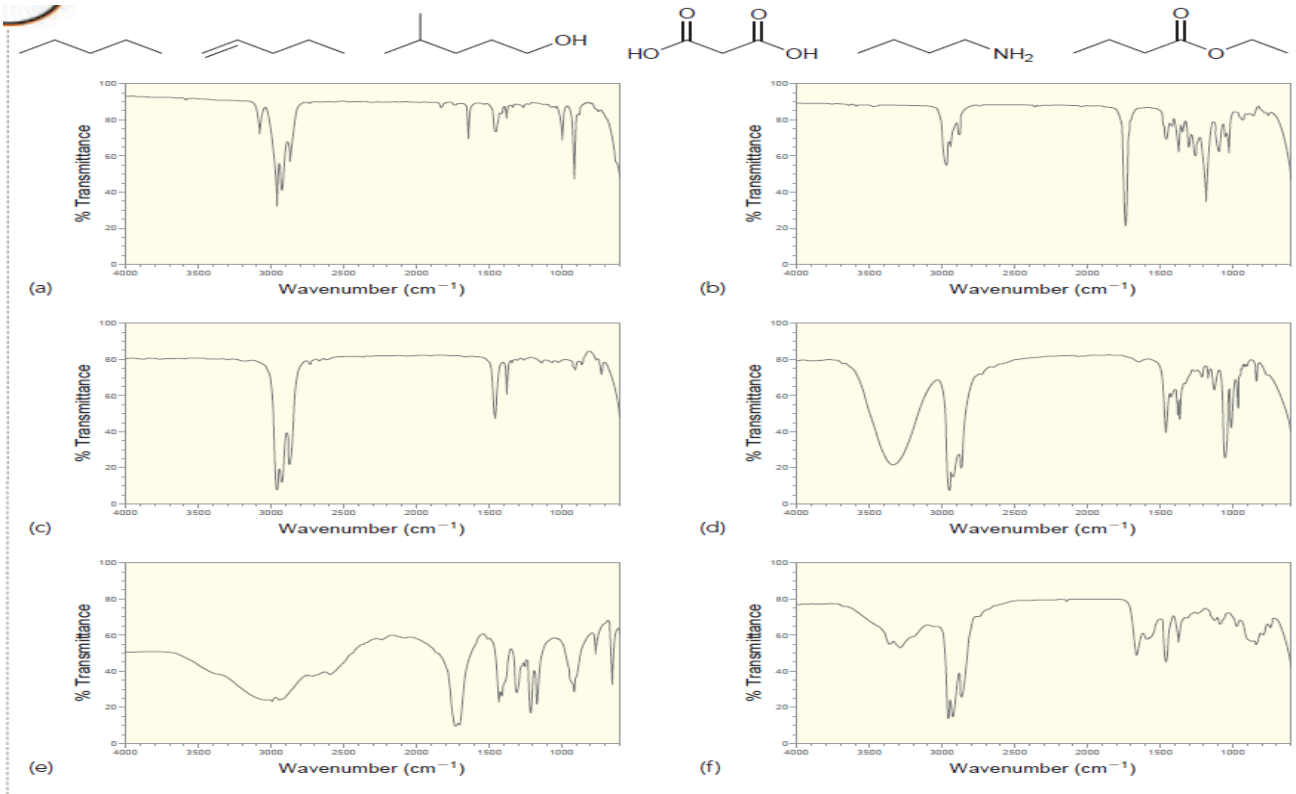
d. $CH_3CH_2C{\equiv}CCH_3$ and $CH_3CH_2C{\equiv}CH$

e.  and

f.  and 

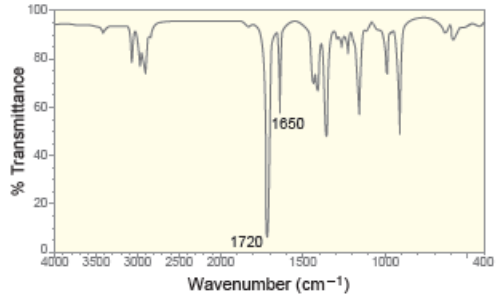
Q7/ When 1-chlorobutane is treated with sodium hydroxide, two products are formed. Identify the two products, and explain how these products could be distinguished using IR spectroscopy.

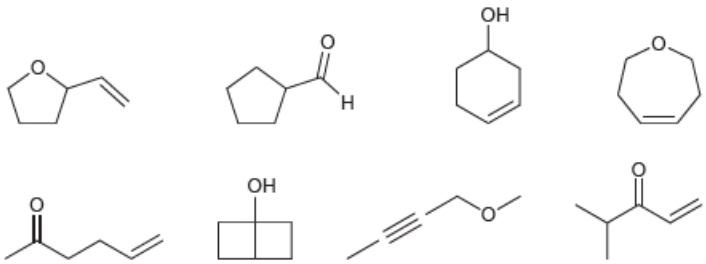
Q8/ Match the expected compound with the appropriate IR spectrum:



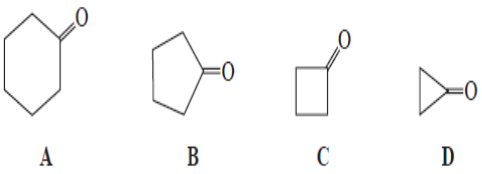
Q9/ A compound with molecular formula C6H10O gives the following IR spectrum.

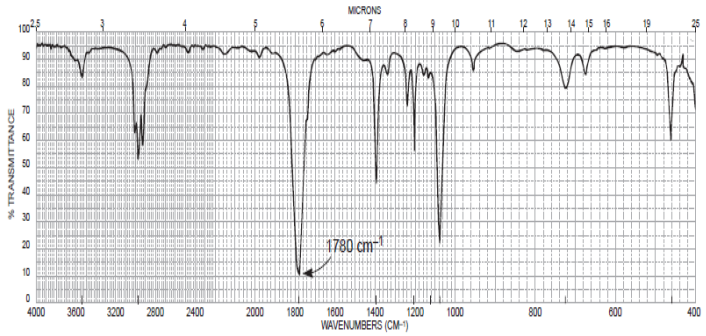
Identify the structure below that is most consistent with the spectrum:

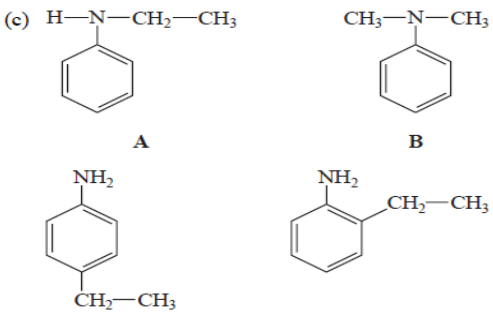


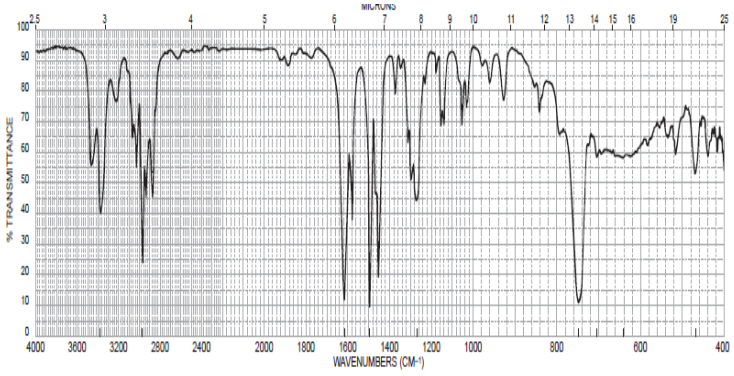


Q10/ Choose the structure that best fits the infrared spectrum shown.









Q11/ An organic compound with molecular mass C8H18 shows the following characteristic

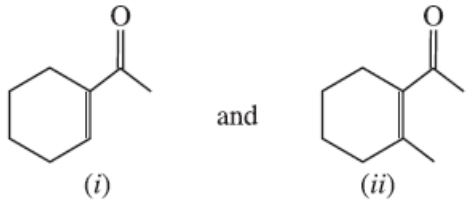
absorption bonds :

(i) 2925 cm–1 (st), (ii) 1465 cm–1, (iii) 1380 cm–1 and (iv) 720 cm–1.

Determine the structure of the compound.

Q12/ The analytical data and the molecular mass determination gave C8H8O as the molecular formula of the compound. The compound burns with a sooty flame and gave an oxime with hydroxylamine hydrochloride. Following absorption bands appear in its Infra-red spectrum : (i) 2825 cm–1, (ii) 2717 cm–1, (iii) 3060 cm–1 and (iv) 1700 cm–1 (s) and 830 cm–1. Deduce the structure of the compound.

Q13/ Which of the following two compounds will show C=O stretching absorption band at a higher wave number? Give suitable reason for your answer.



(*i*) (*ii*)

Q14/ 4: An aromatic organic compound decolourises bromine in carbon tetra-chloride and exhibits the following absorption position.

(i) 3090 cm–1 (ii) 3040 and 3000 cm–1 (iii) 2820 and 2750 cm–1 (iv) 1685 cm–1(s)

(v) 1630 cm–1 (vi) 1580 and 1450 cm–1 (vii) 750 cm–1.

Q15/Can you distinguish a pair of enantiomers by infra-red spectroscopy?

Q16/ What happens to O-H str position when 10 ml of carbon tetrachloride is added to 2 ml of ethyl alcohol?

Q17/ In acetylene, —C≡C—H str. appears at about 3300 cm–1. How will you distinguish it from an O-H str. in alcohol?

Q18/ What is the effect of hybridization of carbon on the stretching frequency of C-H bonds?

Q19/How will you distinguish between *cis* and *trans*-cinnamic acid?

Q20/An organic compound (A) with molecular formula C3H7NO gives absorption peaks in the regions 3413 (*m*), 3236 (*m*), 3030–2899 (*m*), 1667 (*s*), 1634 (*s*) and 1460 cm–1 (*s*). Give its probable structure.

Q21/ Propose four possible structures for a compound C_4H_8O that exhibits a broad signal between 3200

and 3600 cm^{-1} in its IR spectrum and does not contain any signals between 1600 and 1850 cm^{-1}.

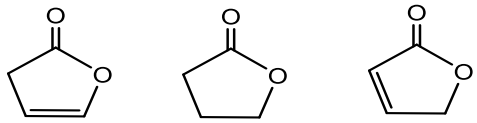
Q22/ Compare the **O-H str.** Position and shape of **non-**, **intra** and **inter-** hydrogen bonded hydroxyl compounds.

Non-hydrogen bonded….

Intra-molecular-hydrogen bonded…..

Intermolecular-hydrogen bonded…..

Q23/ Arrange and explain the following compounds in order of increasing **carbonyl** absorption (cm^{-1}) bands.



p-nitro benzaldehyde, m-nitro benzaldehyde and p-hydroxy benzaldehyde

Q24/ How could IR spectroscopy distinguish among hex-1-yne, hex-2-yne, and hex-3-yne?

Q25/The carbonyl stretching frequency in 2, 4, 6-cycloheptatrienone is exceptionally low. Explain.

Q26/ An aromatic organic compound (C_9H_8O) decolorize bromine and $KMnO_4$ and exhibit the following absorption positions. (*i*) 3090 cm^{-1} (*ii*) 3040 and 3000 cm^{-1} (*iii*) 2820 and 2750 cm^{-1} (*iv*) 1685 cm^{-1}(s) (*v*)

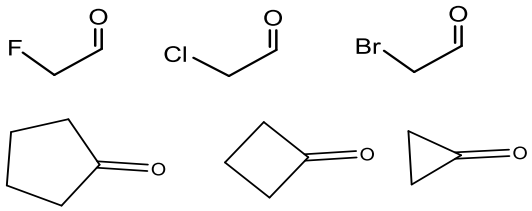
1630 cm^{-1} (*vi*) 1580, 1450 cm^{-1} (*vii*) 690 and 750 cm^{-1}.

Q27/ Propose five possible structures for C_5H_9N that exhibits a sharp signal between 2100-2300 cm^{-1} in its IR spectrum and does not contain any signals between 3000 - 4000 cm^{-1}.

Q28/ Hydrocarbon containing 10% hydrogen show the following bands in its IR spectrum:

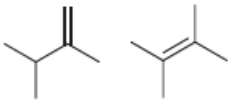
(i) 3295 cm-1 (ii) 2130 cm-1. Deduce the structure of this hydrocarbon.

Q29/ Arrange and explain the following compounds in order of increasing **carbonyl** absorption (cm^{-1}) bands.



ethyl benzoate phenyl ethanoate

Q30/ how could IR spectroscopy distinguish between?

1: 

2: The two isomers of (C_6H_{12}) *trans*-3-hexene and 2,3-dimethyl-2-butene

Q31/ Deduce the structure of organic compound (C_7H_7NO) that exhibit the following absorption positions.

(i) 3370 cm^{-1} (*ii*) 3170 and 3070 cm^{-1} (*iii*) 1670 cm^{-1}(s) (iv) 1630 cm^{-1} (*v*) 690 and 750 cm^{-1}.

Q32/ **How will you distinguish between the following pairs? 4pts**

A: CH3CH2COCl and CH3CH2Cl

B: CH3CH2OH and CH3CH2COOH

Q33/**Match the following compounds with their wave numbers(cm-1) 6pts**

A/ methylacetate, propanone , ethanamide 1715, 1680, 1740

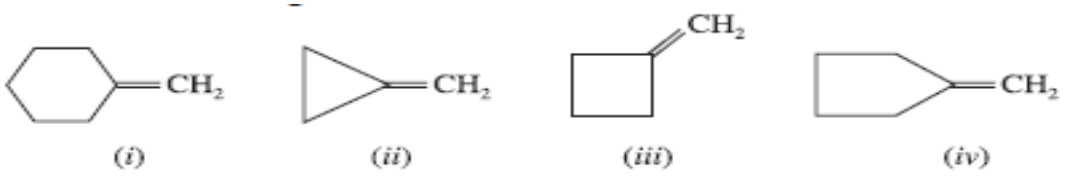
B/ Propyne, propene, propane, pyridine 3100, 3050, 3300, 2960

Q34/ How will you distinguish between o & p-hydroxy benzoic acid by IR spectroscopy?

Q35/ / Compound C8H8O gave an imine with PhNH2 and has the following IR data:

2825, 2717, 3060, 1700 and 830cm-1 Deduce the structure

Q36/ Arrange the following compounds in order of their increasing wave number of absorption due to C=C stretching



Q37/ acetylcyclohexane and 1-acetylcyclohexene ***due to C=Ostretching***

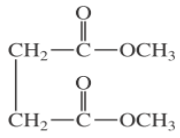
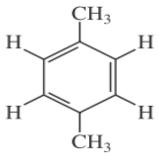
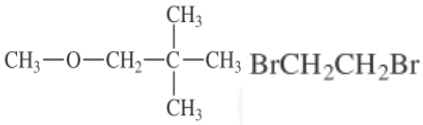
Q38/ An organic compound (A) with molecular formula C3H7NO gives absorption peaks in the regions 3413 (*m*), 3236 (*m*), 3030–2899 (*m*), 1667 (*s*), 1634 (*s*) and 1460 cm^{-1} (*s*). Give its probable structure.

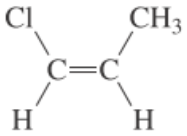
Q39/The carbonyl stretching frequency in 2, 4, 6-cycloheptatrienone is exceptionally low. Explain.

Q40/ Treating 1,2-cyclohexanediol with concentrated sulfuric acid yields a product with molecular formula C6H10O. An IR spectrum of the product exhibits a strong signal at 1720 cm-1. Identify the structure of the product, and show a mechanism for its formation.

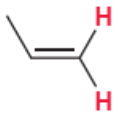
^{1}H-NMR Questions

Q41/ determine the number of signals for each of the following:

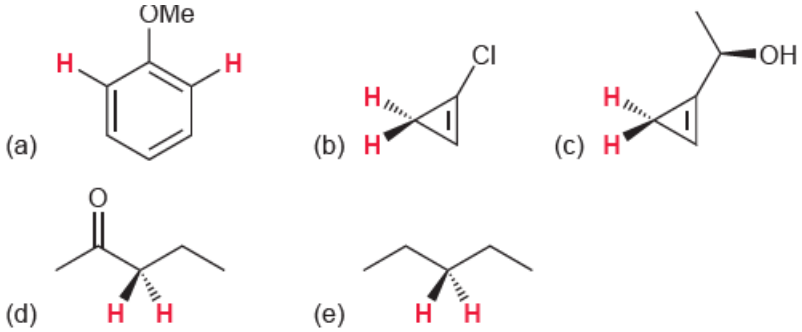






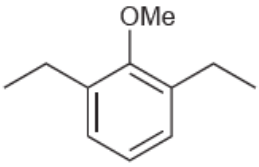
Q42/ Determine whether the two protons shown in red are homotopic, enantiotopic, diastereotopic, or simply not related at all.



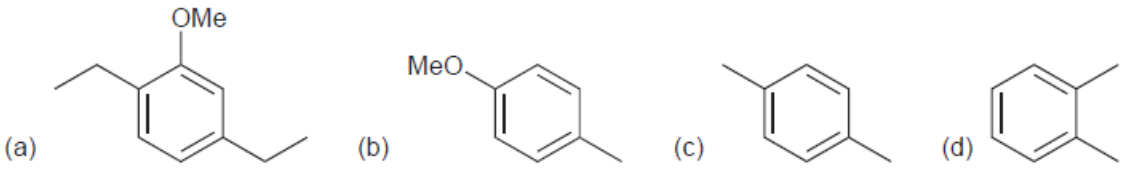
Q43/ For each of the following compounds, determine whether the two protons shown in red are homotopic, enantiotopic, or diastereotopic:



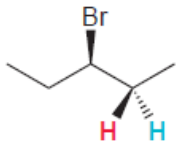
Q44/ Identify the number of signals expected in the 1H NMR spectrum of the following compound.



Q45/ Identify the number of signals expected in the 1H NMR spectrum of each of the following compounds.



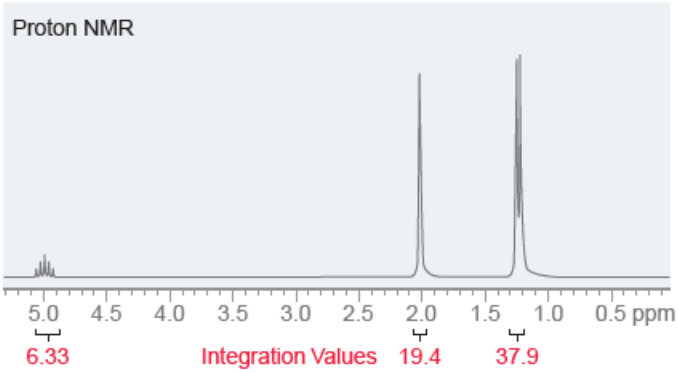
Q46/ We saw a general rule that the two protons of a CH2 group will be chemically equivalent if there are no chirality centers in the compound. An example of an exception is 3-bromopentane. This compound does not possess a chirality center. Nevertheless, the two highlighted protons are not chemically equivalent. Explain.



Q47/ Identify the structure of a compound with molecular formula C9H20 that exhibits four CH2 groups, all of which are chemically equivalent. How many total signals would you expect in the 1H NMR spectrum of this compound?

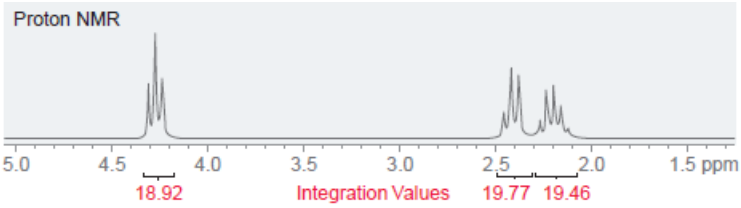
Q48/A compound with molecular formula C5H10O2has the following 1H NMR spectrum.

Determine the number of protons giving rise to each signal.



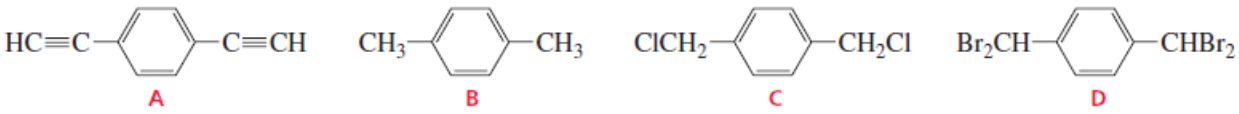
Q49/ A compound with molecular formula C4H6O2 has the following NMR spectrum.

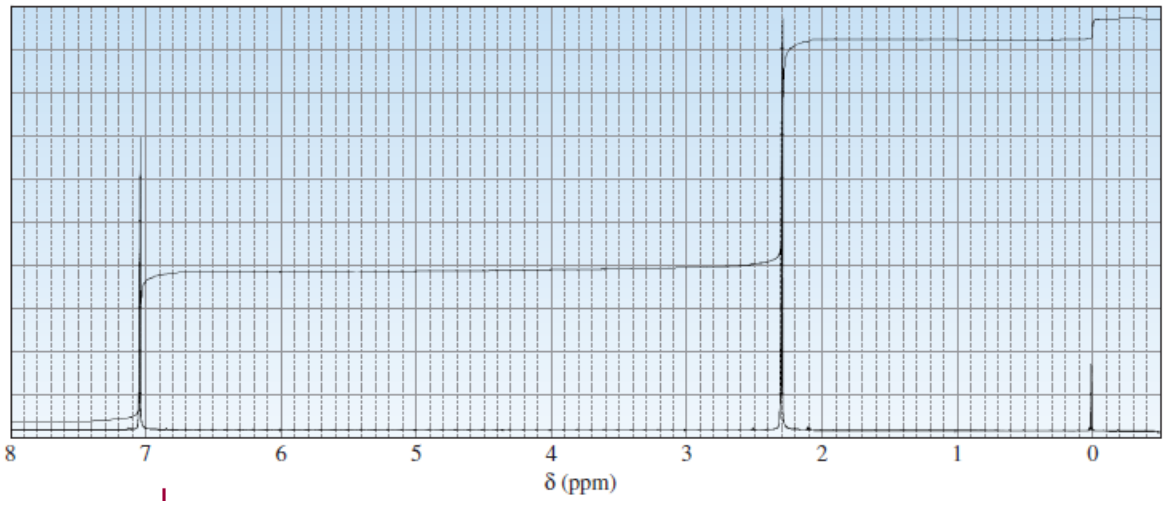
Determine the number of protons giving rise to each signal.



Q50/ The 1H NMR spectrum of a compound with molecular formula C7H15Cl exhibits two signals with relative integration 2 : 3. Propose a structure for this compound.

Q51/The 1H-NMR spectrum shown in Figure corresponds to one of the following compounds. Which compound is responsible for this spectrum?





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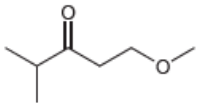
Q52/ Predict the chemical shifts for the signals in the 1H NMR spectrum of the following compound.



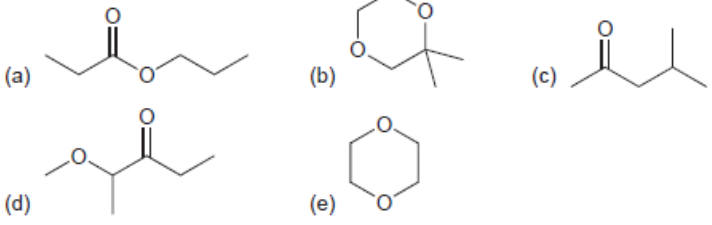
Q53/ which underlined proton has the greater chemical shifts?

a. $CH_3CH_2C\underline{H}_2Cl$ or $CH_3CH_2C\underline{H}_2Br$

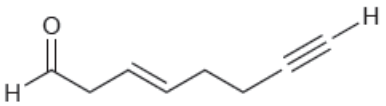
b. $CH_3CH_2C\underline{H}_2Cl$ or $CH_3CH_2C\underline{H}(Cl)CH_3$

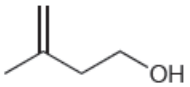
c. $CH_3CH_2\underline{C}(=O)H$ or $CH_3CH_2C(=O)OC\underline{H}_3$

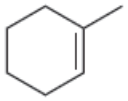
Q54/ Predict the chemical shifts for the signals in the 1H NMR spectrum of each of the following compounds:

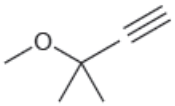


Q55/ For each of the following compounds, identify the expected chemical shift for each type of proton:

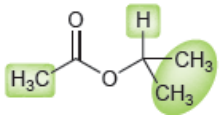
(a) 

(b) 

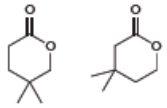
(c) 

(d) 

Q56/ Draw the expected 1H NMR spectrum of isopropyl acetate.



Q57/ Using 1H NMR Spectroscopy to distinguish between Compounds

1. Three constitutional isomers of xylene.
2. 

Q58/ deduce the structure of the following compounds: C_8H_9BrO

Number of signals	1	2	3	4
Chemical shifts	**2.4**	**3.4**	**6.6**	**7.4**
Multiplicity	t	q	d	d
Intensity	6	4	4	4
Ratio	1.5	1	1	1

Q59/ $C_8H_8O_2$

Number of signals	1	2	3	4
Chemical shifts	**10**	**7.7**	**6.8**	**3.8**
Multiplicity	s	d	d	s
Intensity	6	12	12	18
Ratio	1	2	2	3

Q60/ $C_3H_3Cl_5$

t(4.52ppm, 1H), d(6.1ppm, 2H)

Q61/ C_3H_8O

Number of signals	1	2	3	4
Chemical shifts	**0.9**	**1.5**	**2.6**	**3.6**
Multiplicity	t	sextet	s	t
Intensity	3	2	1	2

Q62/ $C_4H_7O_2Br$

Number of signals	1	2	3	4
Chemical shifts	**1.1**	**2.1**	**4.2**	**10.5**
Multiplicity	t	quintet	t	s
Intensity	3	2	1	1

Q63/ a compound with C8H8O give the following NMR data:

Multiplet (7.28ppm, 5H), d(2.8ppm,2H), t(9.7ppm,1H). Deduce the structure.

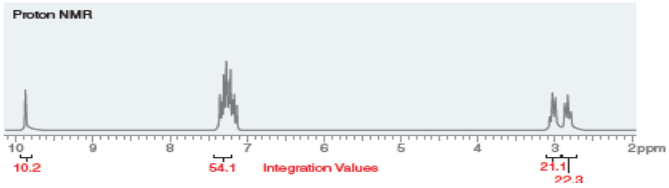
Q64/ a compound with C8H12O give the following NMR data:

s(1.1ppm,6H), s(2.15ppm,3H), s(2.6ppm,2H), s(3.9ppm,1H). Deduce the structure.

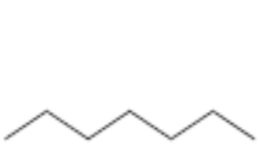
Q65/ a compound with C7H12O give the following NMR data:

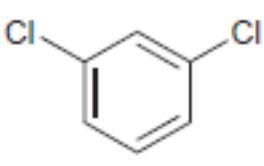
m(1.6ppm,4H), m(1.76ppm,4H), t(2.5ppm,4H). Deduce the structure

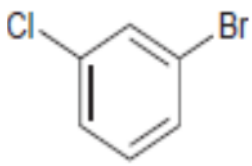
Q66/ Identify the structure of a compound with the molecular formula C9H10O that exhibits the following 1H NMR spectrum:



Q67/ Identify the number of signals expected in the 1H NMR spectrum of each of the following compounds.



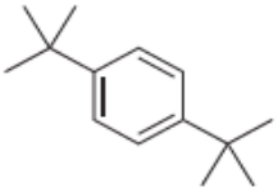


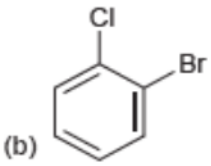


Q68/ the following compounds exhibits 1H NMR spectrum with two signals. Deduce the structure of each compound:

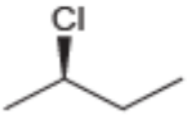
C6H12 , C12H24

Q69/ How many signals would you expect in the 1H NMR spectrum of each of the following compounds:





(b)



Q70/ the following compounds exhibits a 1H NMR spectrum with only one signal. Deduce the structure of each compound:

(b) $C_5H_8Cl_4$ (c) $C_{12}H_{18}$

Q71/ deduce structure of C6H10O3

Number of signals	1	2	3	4
Chemical shifts	1.2	2.2	3.5	4.1
Multiplicity	t	s	s	q
Intensity	5.9	5.4	3.5	4

Q72/ Compound C7H5OCl3 show singlet at 3.9(3H), and two d[7.3(1H)and 6.75(1H)]

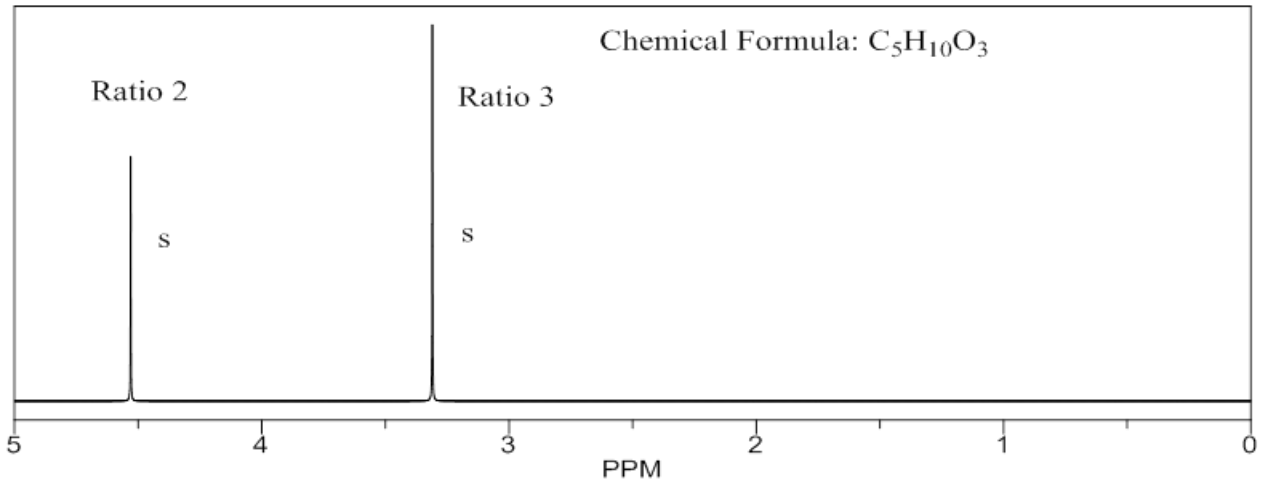
Deduce the structure

Q73/ A compound with molecular formula C10H10O4 produces a 1H NMR spectrum that exhibits only two signals, both singlets. One signal appears at 3.9 ppm with a relative integration value of 79. The other signal appears at 8.1 ppm with a relative integration value of 52. Identify the structure of this compound.

Q74/ There are four esters with the molecular formula C4H8O2, draw the structure of the two isomers where the first gives three and the second four signals.

Q75/ Identify the following compound from the NMR data and molecular formula. C4H8Br2, 1.97 ppm (6H) singlet 3.89 ppm (2H) singlet.

Q76/ Identify the following compound from the spectrum:



Q77/ There are five ethers with the molecular formula C5H12O2, draw the structure of the two isomers where the first gives two and the second four signals

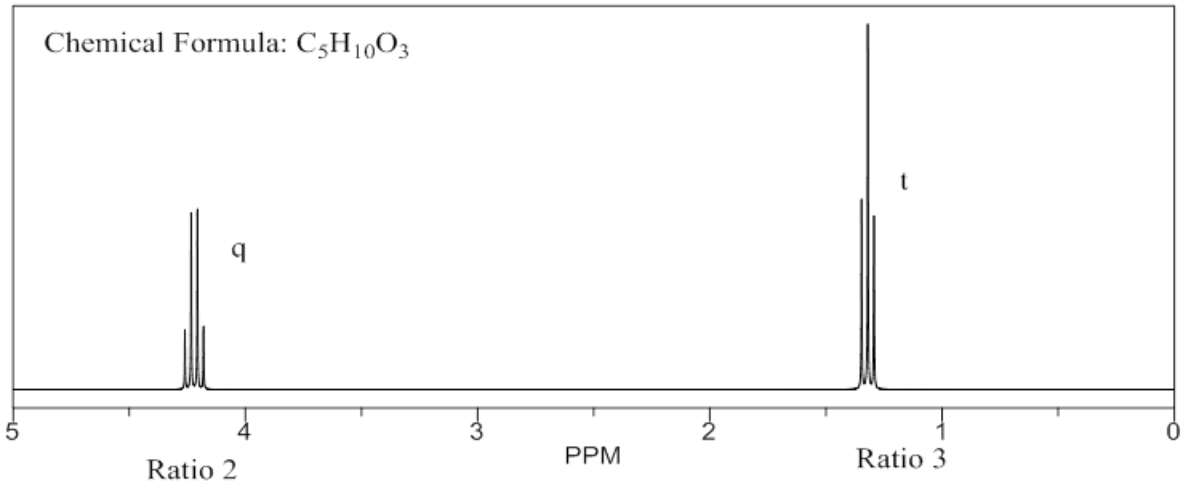
Q78/ An unknown compound has the molecular formula C9H11Br. Its proton NMR spectrum shows the following signals:

singlet, 7.1ppm, integral 44 mm

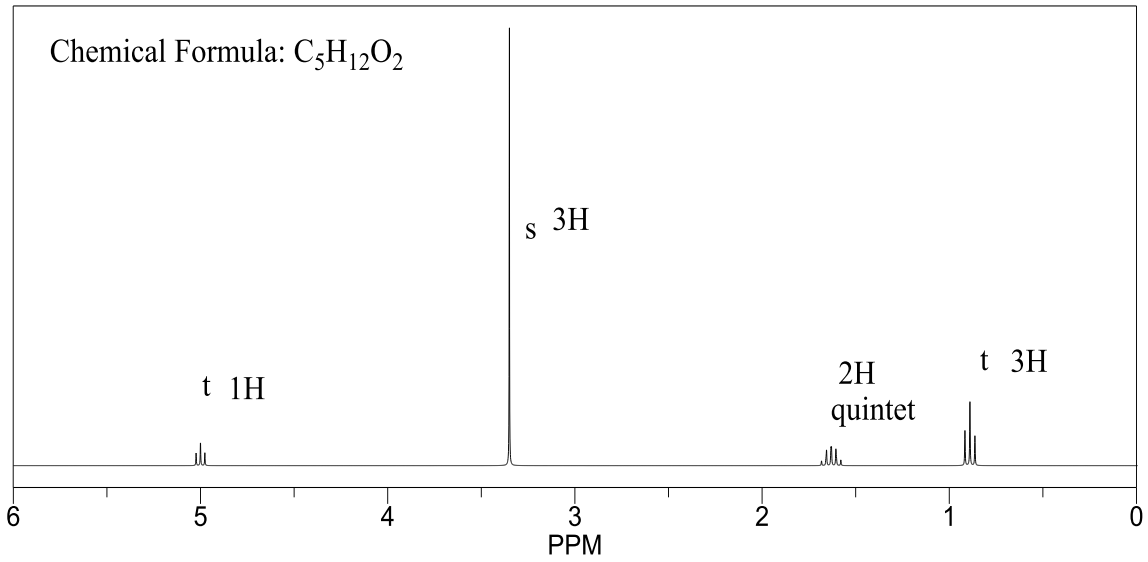
singlet, 2.3ppm, integral 130 mm

singlet, 2.2ppm , integral 67 mm

Q79/ Draw the structure from the spectrum:



Q80/ Draw the structure from the spectrum:



UV-Visible Questions

Q81/ What is the effect of ultra-violet or visible light on the organic compound?

Q82/ What is the effect of hydrogen bonding on ultra-violet absorption?

Q83/ What do you mean by a good solvent in UV spectroscopy and what is its effect on absorption maximum?

Q84/ Describe the shift in absorption (n-π*) when a more polar solvent is used.

Q85/ How will you distinguish between cis and trans-1, 3, 5-Hexatriene.

Q86/ What structural features may produce bathochromic or hypsochromic effect in an organic compound?

Q87/ Define the following terms : (i) Bathochromic shift (ii) Hypsochromic shift (iii) A Chromophore (iv) Hyperchromic effect.

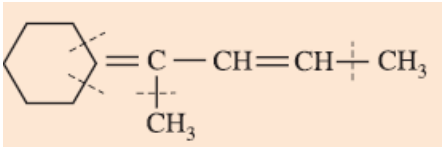
Q88/ Aniline absorbs at 280 nm however, in acidic solution, the main absorption band is seen at 203 nm. Explain.

Q89/Calculate the absorption maximum in the ultra-violet spectrum of 2, 4- Hexadiene.

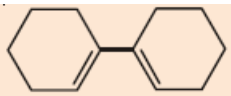
SOLUTION: The basic unit in 2, 4. hexadiene is butadiene. There are two alkyl substituents (one on each double bond) on it. Thus,

(CH3—CH=CH—CH=CH—CH3)

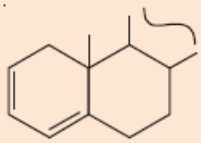
Q90/ *Calculate the absorption maximum in the UV spectrum of*



Q91/ *Calculate λ_{max} for*

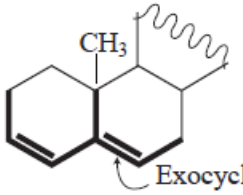


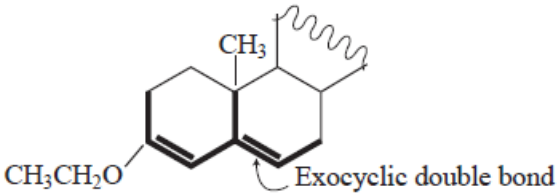
Q92/ *Calculate the absorption maximum for the compound*



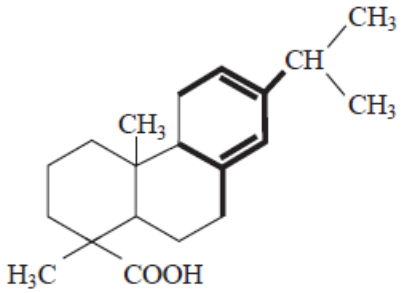
in ethanol.

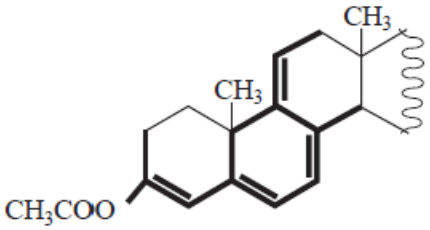
Q93/ Calculate λ max of:



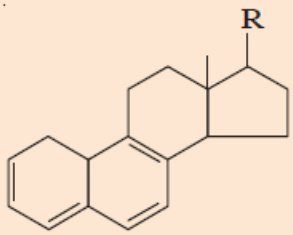


Q94/ Calculate λ max of:

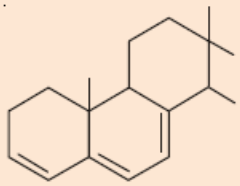




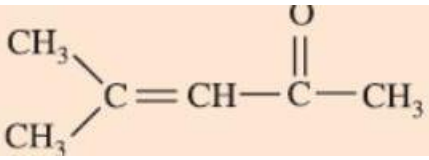
Q95/ *Calculate the value of absorption maximum for the compound*



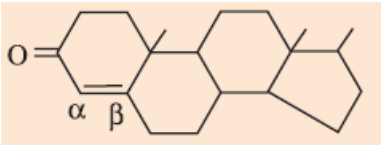
Q96/ *Calculate λ_{max} for the compound.*



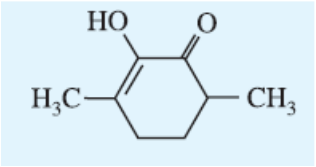
Q97/Calculate λmax of



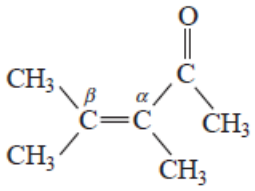
Q98/

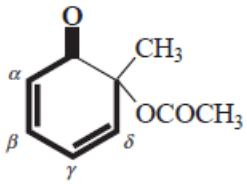


Q99/

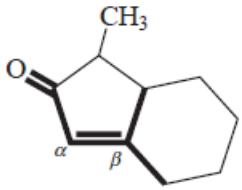


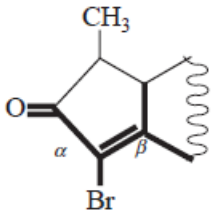
Q100/



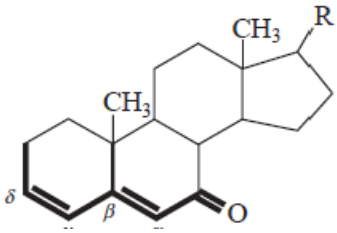


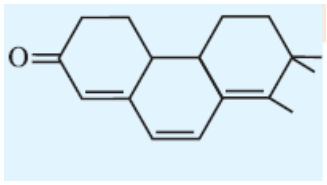
Q101/

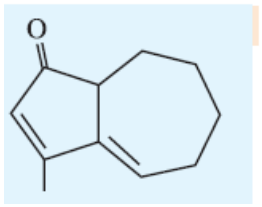


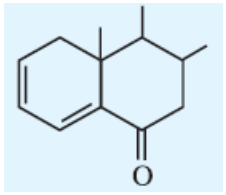


Q102/

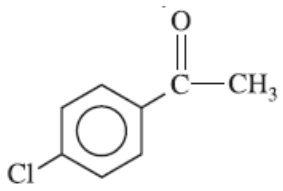


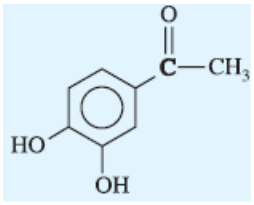
Q103/ 

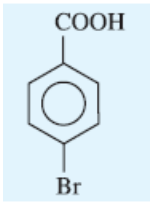
Q104/ 

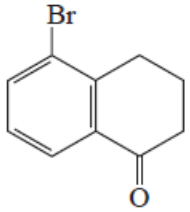
Q105/ 

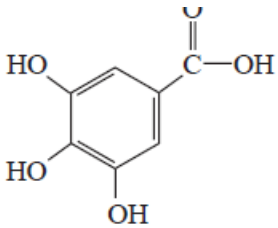
Q106/ Calculate the absorption maximum in ethanol for p-chloroacetophenone.



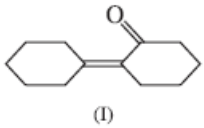
Q107/ Calculate the absorption maximum of 

Q108/ Calculate the absorption maximum of 

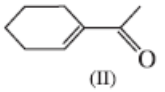
Q109/ 



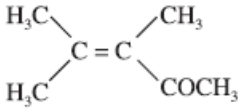
Q110/ Following four ketones are filled in four bottles and their labels are removed. Measurement of ultra-violet spectra of the contents of four bottles give λmax 221, 249, 237 and 258 nm. Assign structures to the appropriate λmax.



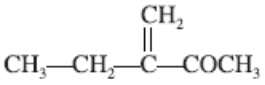
(I)



(II)

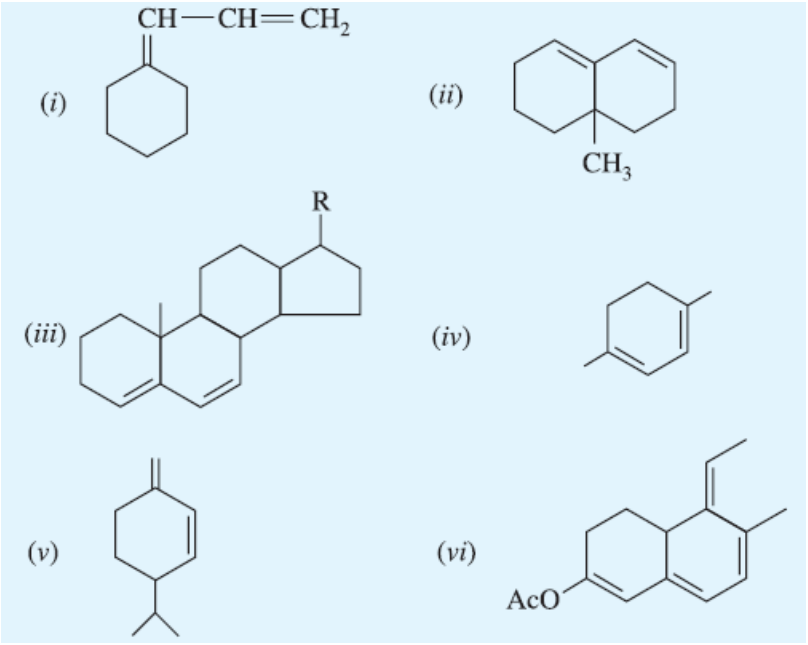


(III)



(IV)

Q111/ Following the Woodward-Fieser rules, calculate the absorption maximum for each of the following compounds



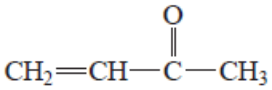
Q112/ Draw structural formulas that are consistent with the following observations:

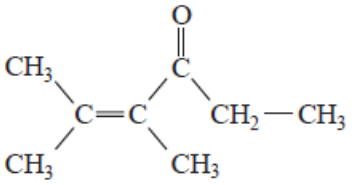
(a) An acid C7H4O2Cl2 shows a UV maximum at 242 nm.

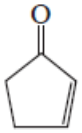
(b) A ketone C8H14O shows a UV maximum at 248 nm.

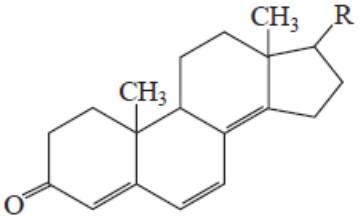
(c) An aldehyde C8H12O absorbs in the UV with lmax = 244 nm.

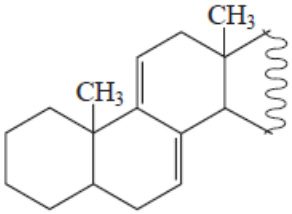
Q113/ Predict the UV maximum for each of the following substances:

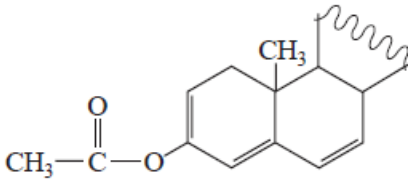
(a) 

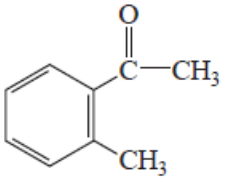
(b) 

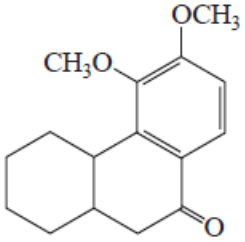
(c) 

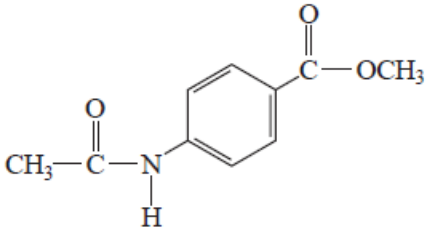
(d) 

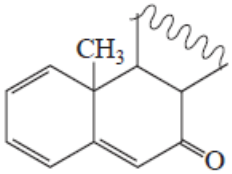
(e) 

(f) 

(g) 

(h) 

(i) 

(j) 

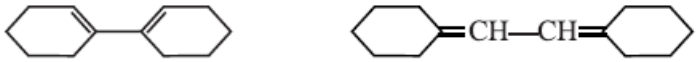
Q114/ The UV spectrum of acetone shows absorption maxima at 166, 189, and 279 nm. What type of transition is responsible for each of these bands?

Q115/ Chloromethane has an absorption maximum at 172 nm, bromomethane shows an absorption at 204 nm, and iodomethane shows a band at 258 nm. What type of transition is responsible for each band? How can the trend of absorptions be explained?

Q116/ What types of electronic transitions are possible for each of the following compounds?

A: Cyclopentene (b) Acetaldehyde (c) Dimethyl ether (d) Methyl vinyl ether (e) Triethylamine (f) Cyclohexane

Q117/ Why the λ_{max} for the diene (I) is observed at lower nm than II?

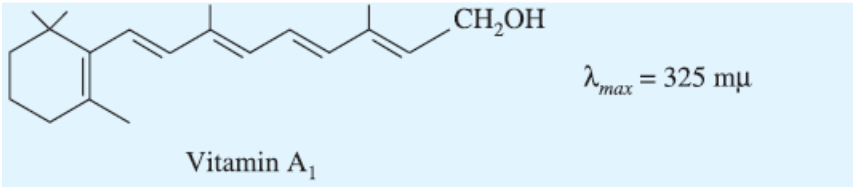


(I) (II)

Q118/ Calculate λmax of:

Lycopene, β-Carotene

Q119/



Vitamin A_1

Q120/