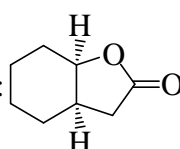
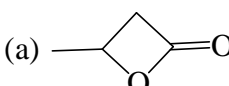
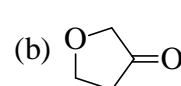
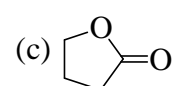
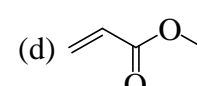
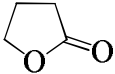
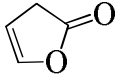
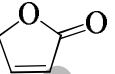
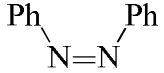
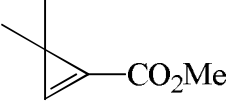
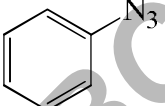
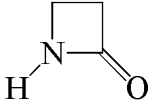
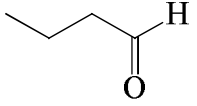
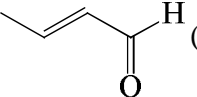
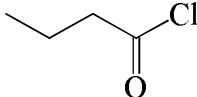
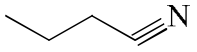


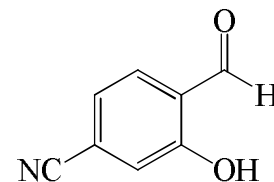
Organic Spectroscopy

- In a 200 MHz NMR spectrometer, a molecule shows two doublets separated by 2 ppm. The observed coupling constant is 10 Hz. The separation between these two signals and the coupling constant in a 600 MHz spectrometer will be, respectively:
 - 600 Hz and 30 Hz
 - 1200 Hz and 30 Hz
 - 600 Hz and 10 Hz
 - 1200 Hz and 10 Hz
- A molecule, AX, has a vibrational energy of 1000 cm^{-1} and rotational energy of 10 cm^{-1} . Another molecule, BX, has a vibrational energy of 400 cm^{-1} and rotational energy of 40 cm^{-1} . Which one of the following statements about the coupling of vibrational and rotational motion is true:
 - The coupling is stronger in BX.
 - The coupling is stronger in AX.
 - Magnitude of coupling is same in both AX and BX.
 - There is no coupling in both AX and BX.
- The order of carbonyl stretching frequency in the IR spectra of ketone, amide and anhydride is:
 - Anhydride > amide > ketone
 - Ketone > amide > anhydride
 - Amide > anhydride > ketone
 - Anhydride > ketone > amide
- In the IR spectrum, carbonyl absorption band for the following compound appears at:
 
 - 1810 cm^{-1}
 - 1770 cm^{-1}
 - 1730 cm^{-1}
 - 1690 cm^{-1}
- In the IR spectrum of p-nitrophenyl acetate, the carbonyl absorption band appears at:
 - 1670 cm^{-1}
 - 1700 cm^{-1}
 - 1730 cm^{-1}
 - 1760 cm^{-1}
- A triatomic molecule of the type AB_2 shows two IR absorption lines and one IR-Raman line. The structure of the molecule is:
 - $\text{B}-\text{B}-\text{A}$
 - $\text{B}-\text{A}-\text{B}$
 - $\text{B}-\text{B}-\text{A}$
 - $\text{B}-\text{A}-\text{B}$
- In the IR spectrum, the absorption band due to carbonyl group in phenyl acetate appears at:
 - 1800 cm^{-1}
 - 1760 cm^{-1}
 - 1710 cm^{-1}
 - 1660 cm^{-1}
- In the IR spectrum of p-nitrophenyl acetate, the carbonyl absorption band appears at:
 - 1660 cm^{-1}
 - 1700 cm^{-1}
 - 1730 cm^{-1}
 - 1770 cm^{-1}
- A compound with molecule formula $\text{C}_4\text{H}_6\text{O}_2$ shows band at 1170 cm^{-1} in IR spectrum and peaks at 178, 68, 28 and 22 ppm in ^{13}C NMR spectrum. The correct structure of the compound is:
 - 
 - 
 - 
 - 

10. The compound that exhibits sharp bands at 3300 and 2150 cm^{-1} in the IR spectrum is:
 (a) 1-butyne (b) 2-butyne (c) Butyronitrile (d) Butylamine
11. The resonance Raman stretching frequency ($\nu_{\text{o-o}}$, cm^{-1}) of O_2 is 1580 . The $\nu_{\text{o-o}}$ for O_2 in bond oxy-hemoglobin is close to:
 (a) 1600 (b) 1900 (c) 800 (d) 1100
12. Correctly matched structure and carbonyl stretching frequency set is:
- | | | | |
|-------------------|---|--|---|
| Column – A | (P)  | (Q)  | (R)  |
| Column – B | (X) 1750 cm^{-1} | (Y) 1770 cm^{-1} | (Z) 1800 cm^{-1} |
| (a) P-Y, Q-Z, R-X | (b) P-Y, Q-X, R-Z | (c) P-Z, Q-Y, R-X | (d) P-X, Q-Z, R-Y |
13. Among the following, the compound that displays an IR band at 2150 cm^{-1} is:
 (a)  (b)  (c)  (d) 
14. The compound which shows IR frequencies at both 3314 and 2126 cm^{-1} is:
 (a) $\text{CH}_3(\text{CH}_2)_4\text{CH}_2\text{SH}$ (b) $\text{CH}_3(\text{CH}_2)_4\text{CH}_2\text{C}\equiv\text{N}$
 (c) $\text{CH}_3(\text{CH}_2)_4\text{CH}_2\text{C}\equiv\text{C}-\text{H}$ (d) $\text{CH}_3(\text{CH}_2)_2\text{C}\equiv\text{C}(\text{CH}_2)_2\text{CH}_3$
15. Match the compound P-S with their carbonyl stretching frequencies (cm^{-1}) I-VI in IR spectroscopy.
- | | |
|--------------------|-------------|
| P. Acetone | I. 1870 |
| Q. Ethyl acetate | II. 1800 |
| R. Acetamide | III. 1740 |
| S. Acetyl chloride | IV. 1700 |
| | V. 1660 |
| | VI. 1600 |
- (a) P-IV, Q-III, R-I, S-VI (b) P-III, Q-VI, R-V, S-II
 (c) P-IV, Q-III, R-V, S-II (d) P-II, Q-V, R-III, S-VI
16. Out of the following, the one which is not an excitation source for IR spectrometer is:
 (a) Tungsten filament lamp (b) Nernst glower
 (c) Deuterium lamp (d) Mercury arc
17. The molecule active in rotation microwave, infrared absorption as well as rotational Raman spectra is:
 (a) CO_2 (b) SF_6 (c) HCl (d) H_2
18. Match the compounds in List – I with the stretching frequencies (cm^{-1}) of the principal functional groups given in List – II.
- | | | | | |
|---------------------------|---|---|--|---|
| List – I | (1)  | (2)  | (3)  | (4)  |
| List II | (I) 2240 | (II) 1795 | (III) 1750 | (IV) 1695 |
| (a) 1-III, 2-IV, 3-I, 4-V | (b) 1-III, 2-IV, 3-II, 4-V | (c) 1-IV, 2-V, 3-II, 4-I | (d) 1-IV, 2-III, 3-V, 4-I | |

19. The IR stretching frequencies (cm^{-1}) for the compound X are as follows: 3300-3500 (s, br); 3000

(m); 2225 (s); 1680(s). The correct assignment of the absorption bands is:



(a) $\bar{\nu}_{(\text{OH})} = 3300 - 3500$; $\bar{\nu}_{(\text{CH})} = 3000$; $\bar{\nu}_{(\text{CN})} = 2225$; $\bar{\nu}_{(\text{CO})} = 1680$

(b) $\bar{\nu}_{(\text{OH})} = 3000$; $\bar{\nu}_{(\text{CH})} = 3300 - 3500$; $\bar{\nu}_{(\text{CN})} = 2225$; $\bar{\nu}_{(\text{CO})} = 1680$

(c) $\bar{\nu}_{(\text{OH})} = 3300 - 3500$; $\bar{\nu}_{(\text{CH})} = 3000$; $\bar{\nu}_{(\text{CN})} = 1680$; $\bar{\nu}_{(\text{CO})} = 2225$

(d) $\bar{\nu}_{(\text{OH})} = 3000$; $\bar{\nu}_{(\text{CH})} = 3300 - 3500$; $\bar{\nu}_{(\text{CN})} = 1680$; $\bar{\nu}_{(\text{CO})} = 2225$

20. Among the compounds given in the option (a) to (d), the one that exhibits a sharp band at around 3300 cm^{-1} in the IR spectrum is:

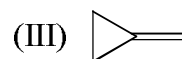
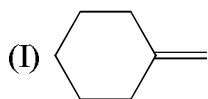
(a) 1, 2-butadiene

(b) 1, 3-butadiene

(c) 1-butyne

(d) 2-butyne

21. The correct order of IR stretching frequency of the C=C in the following olefins is:



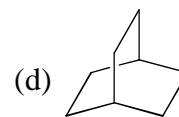
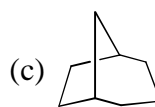
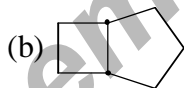
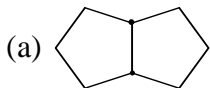
(a) I > II > III

(b) II > III > I

(c) III > II > I

(d) III > I > II

22. Proton decoupled ^{13}C NMR spectrum of a bicyclooctane (C_8H_{14}) exhibits only two signals. The structure of the compound is:



23. What are the limits of detection of the following common analytical methods used with capillary separations: fluorescence, mass spectrometry, UV-Vis absorbance, and NMR, respectively, in mol:

(a) 10^{-18} - 10^{-23} , 10^{-13} - 10^{-21} , 10^{-13} - 10^{-16} , 10^{-9} - 10^{-11} (b) 10^{-13} - 10^{-21} , 10^{-18} - 10^{-23} , 10^{-13} - 10^{-16} , 10^{-9} - 10^{-11}

(c) 10^{-18} - 10^{-23} , 10^{-13} - 10^{-21} , 10^{-9} - 10^{-11} , 10^{-13} - 10^{-16} (d) 10^{-13} - 10^{-21} , 10^{-13} - 10^{-16} , 10^{-18} - 10^{-23} , 10^{-9} - 10^{-11}

24. Of the molecules CH_4 , CO_2 , benzene and H_2 , the ones that will absorb infrared radiation are:

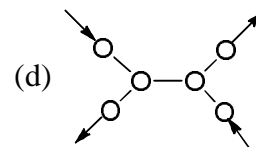
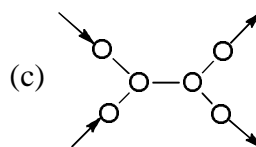
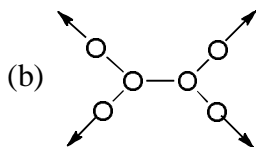
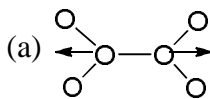
(a) CH_4 , CO_2 , benzene

(b) CH_4 , benzene and H_2

(c) CO_2 , benzene and H_2

(d) CH_4 , CO_2 and H_2

25. Which one of the normal modes of ethylene is active in the infrared:



26. The vibrational stretching frequency of N_2 can be determined using:

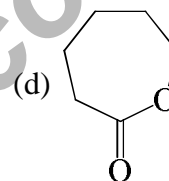
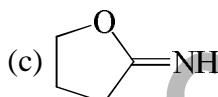
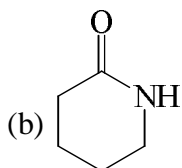
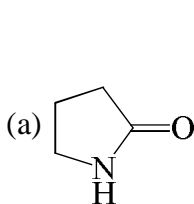
(a) Infrared spectroscopy

(b) Microwave spectroscopy

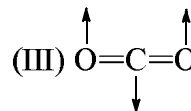
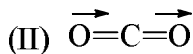
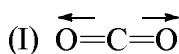
(c) Raman spectroscopy

(d) Rotational Raman spectroscopy

27. The number of IR active vibrational modes in ammonia is:
 (a) 6 (b) 4 (c) 2 (d) 3
28. The number of vibrational degree of freedom in a gaseous mixture of $^{35}\text{Cl}_2\text{O}$, $^{37}\text{Cl}_2\text{O}$, and ^{35}Cl , ^{37}ClO is:
 (a) 1 (b) 2 (c) 3 (d) 4
29. IR stretching frequencies of carbonyl groups in aldehydes and acid chlorides in cm^{-1} are:
 (a) 1730 – 1700 and 1650 – 1580 (b) 1680 – 1660 and 1730 – 1700
 (c) 1730 – 1700 and 1820 – 1770 (d) 1680 – 1660 and 1820 – 1770
30. Which among the following exhibits a carbonyl absorption band at 1770 cm^{-1} :

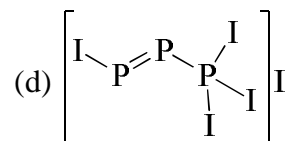
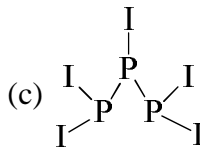
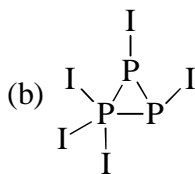
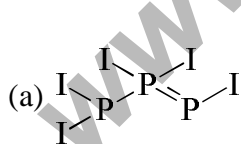


31. Which one of the following exhibits rotational spectra:
 (a) H_2 (b) N_2 (c) CO (d) CO_2
32. The bond that gives the most intense band in the infrared spectrum for its stretching vibrations is:
 (a) C—H (b) N—H (c) O—H (d) S—H
33. An examinations of saturated hydrocarbons containing methyl group show asymmetrical (V_{as}) and symmetrical (V_s) stretching modes in the region of:
 (a) 2960 and 2870 cm^{-1} (b) 3200 and 3100 cm^{-1}
 (c) 1800 and 1700 cm^{-1} (d) 1650 and 1450 cm^{-1}
34. ^{13}C NMR spectrum of DMSO-d_6 gives a signal at $\delta 39.7\text{ ppm}$ as a:
 (a) Singlet (b) Triplet (c) Quintet (d) Septet
35. The molecule with the smallest rotational constant (in the microwave spectrum) among the following is:
 (a) $\text{N} \equiv \text{CH}$ (b) $\text{HC} \equiv \text{CCl}$ (c) $\text{CCl} \equiv \text{CF}$ (d) $\text{B} \equiv \text{CCl}$
36. Of the vibrational modes given below, the IR active mode(s) is (are):

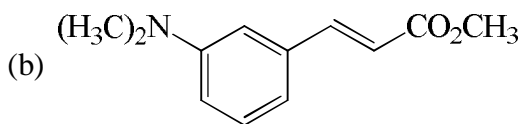
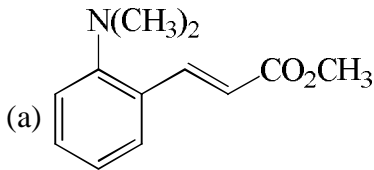


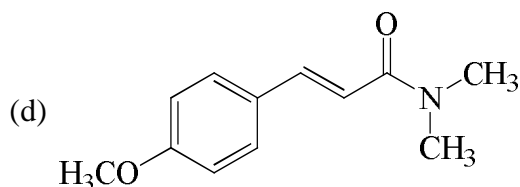
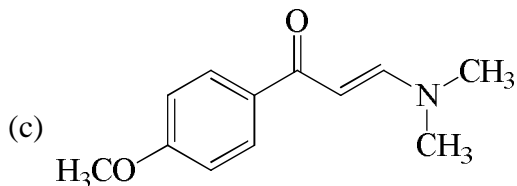
- (a) II only (b) III only (c) I and II (d) II and III
37. Which of the following statements is/are true:
 (I) HCl absorbs IR radiation (II) CO_2 absorbs IR radiation
 (III) H atom absorbs IR radiation
 (IV) H atom absorbs UV- vis and microwave radiation
 (a) I only (b) I and II (c) I, II and III (d) I, II and IV

38. N_2 does not show pure vibrational spectral because:
- (a) Triple bond in N_2 is very strong (b) The dipole moment of N_2 is zero
 (c) Both a and b (d) None of the above.
39. How many normal modes does the CO_2 molecule have; What if the C and the O atoms were constrained to move in one dimensional:
- (a) 4 normal modes for free CO_2 and 4 for constrained CO_2
 (b) 3 normal modes for free CO_2 and 2 for constrained CO_2
 (c) 3 normal modes for free CO_2 and 3 for constrained CO_2
 (d) 4 normal modes for free CO_2 and 2 for constrained CO_2
40. 1H NMR spectrum of a mixture of benzene and acetonitrile shows two singlets of equal integration. The molar ratio of benzene: acetonitrile is:
- (a) 1:1 (b) 2:1 (c) 1:2 (d) 6:1
41. The absorption at λ_{max} 279 nm ($\epsilon = 15$) in the UV spectrum of acetone is due to:
- (a) $\pi-\pi^*$ transition (b) $n-\pi^*$ transition (c) $\sigma-\sigma^*$ transition (d) $\pi-\sigma^*$ transition
42. 1H NMR spectrum of an organic compound recorded on a 500 MHz spectrometer showed a quartet with line positions at 1759, 1753, 1747, 1741 Hz. Chemical shift (δ) and coupling constant (Hz) of the quartet are:
- (a) 3.5 ppm, 6Hz (b) 3.5 ppm, 12 Hz (c) 3.6 ppm, 6 Hz (d) 3.6 ppm, 12 Hz
43. The correct statement in the context of NMR spectroscopy is:
- (a) Static magnetic field is used to induce transition between the spin states.
 (b) Magnetization vector is perpendicular to the applied static magnetic field.
 (c) The static magnetic field is used to create population difference between the spin states.
 (d) Static magnetic field induces spin-spin coupling
44. The reaction between PI_3 , $PSCl_3$ and zinc powder gives P_3I_5 as one of the products. The solution state ^{31}P NMR spectrum of P_3I_5 shows a doublet (δ 98) and a triplet (δ 102). The correct structure of P_3I_5 is:

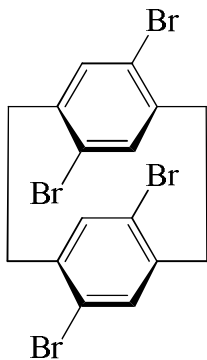


45. The compound that exhibits following spectral data is:
- 1H NMR: δ 8.0 (d, $J = 12.3$ Hz, 1H), 7.7 (d, $J = 8.0$ Hz, 2H), 6.8 (d, $J = 8.0$ Hz, 2H), 5.8 (d, $J = 12.3$ Hz, 1H), 3.8 (s, 3H), 3.0 (s, 6H) ppm

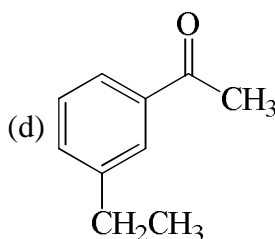
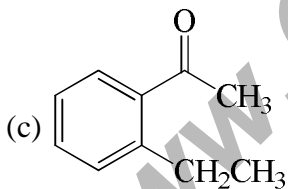
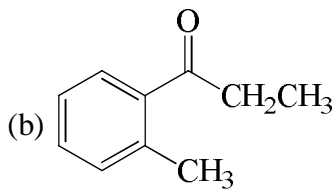
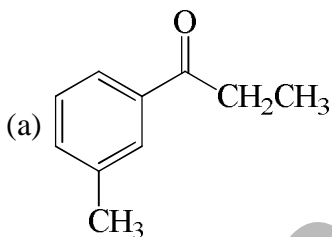




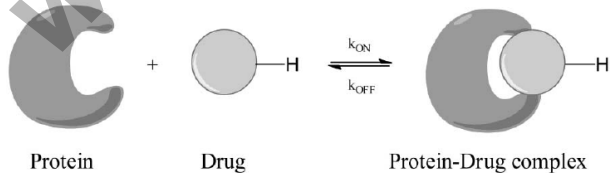
46. Number of signals present in the proton decoupled ^{13}C NMR spectrum of the following compound is:



- (a) Four (b) Six (c) Eight (d) Ten
47. The structure of the compound having the following characteristics spectral data, is IR: 1690 cm^{-1} .
 $^1\text{H-NMR}$: 1.30 (3H, t, $J = 7.2\text{ Hz}$); 2.41 (2H, q, $J = 7.2\text{ Hz}$); 2.32 (3H, s); 7.44 (1H, t, $J = 7.0\text{ Hz}$); 7.57 (1H, dt, $J = 7.0, J = 7.0, 3.0\text{ Hz}$); 7.77 (1H, t, $J = 3.0\text{ Hz}$); 7.90 (1H, dt, $J = 7.0, 3.0\text{ Hz}$); EI mass: m/z 119 (100%); 57 (80%)



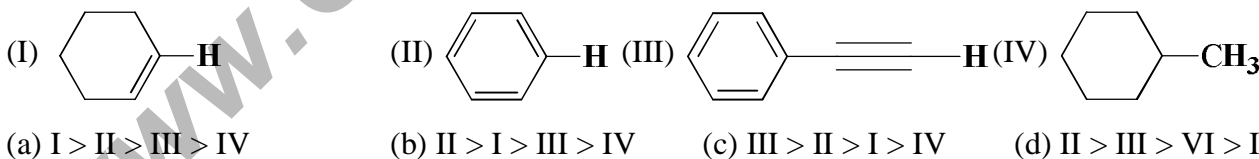
48.



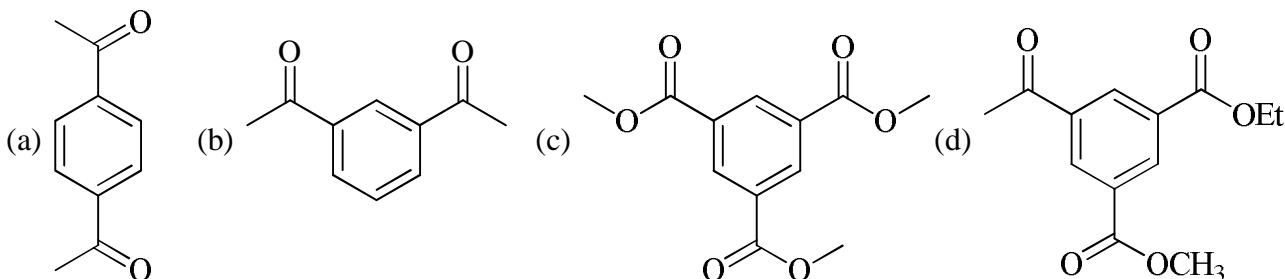
NMR spectroscopy can be used to assay for drug binding to certain protein targets. One of the primary objective of any binding assay is the quantification of the free and the bound forms of a drug molecule at a certain concentration of the protein target. Let us assume that the fully bound drug exhibits a ^1H chemical shift of δ_A while that of the free from resonated at δ_B for the same proton (see

figure above). If the exchange timescale (i.e. proportional to k_{OFF} as k_{ON} is diffusion limited) between the free form of the drug and its bound form is in microseconds, which of the following statements cannot be true assuming that the drug is only 50% bound with its protein target:

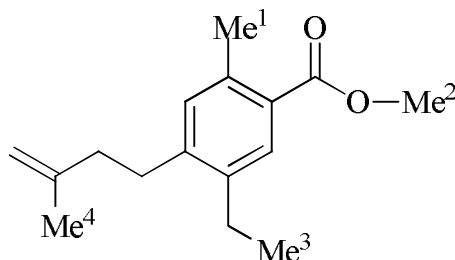
- (a) The NMR line width of the observed transition(s) will be different from the free form of the drug
 (b) There will be two resonance obtained in the NMR spectrum of the Protein-Drug complex: One for the free form while other for the bound form.
 (c) We will see a single resonance at a position δ_{eff} which in between δ_A and δ_B
 (d) Varying the concentration of the drug molecule while observing the NMR signatures will provide an estimate of the binding constant.
49. A compound with molecule formula $C_5H_{12}O_2$ has strong infrared absorption at 3300 to 3400 cm^{-1} . The 1H NMR spectrum showed three singlet at δ 3.45 and δ 3.20 ppm; with relative 3:2:1. Addition of D_2O to the sample eliminates the lower field signal. The ^{13}C NMR spectrum shows three signals all higher than δ 100 ppm. Which of the following compounds best fits this data:
- (a) 1, 5-pentanedial (b) 1, 3-dimethoxypropene
 (c) 2, 2-dimethyl-, 3-prpanediol (d) 2, 4-pentanediol
50. The optimized variation wave functions gives:
- (a) All properties and energy of same quality (b) Properties better than the energy
 (c) Energy better than properties (d) Equal kinetic and potential energy values.
51. The spectroscopic data for an organic compound with molecular formula $C_{10}H_{12}O_2$ are given below. IR band around 1750 cm^{-1} . 1H NMR δ 7.3 (m, 5H), 5.85 (q, 1H, $J = 7.2\text{ Hz}$), 2.05 (s, 3H), 1.5 (d, 3H, $J = 7.2\text{ Hz}$) ppm. The compound is:
- (a) Methyl 2-phenylpropionate (b) 1-(phenylethyl) acetate
 (c) 2-(phenylethyl) acetate (d) Methyl 3-phenylpropionate
52. The correct order of the 1H NMR chemical shift values (δ) for the indicated hydrogens (in bold) in the following compounds is:



53. Which of the following compound show only two signals in 1H NMR and a strong IR bond at $\sim 1690\text{ cm}^{-1}$:

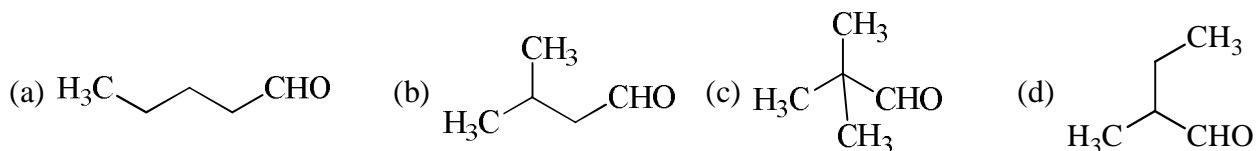


54. The correct order of ^1H NMR chemical shift (δ) values for the labeled methyl groups in the following compound is:



- (a) $\text{Me}^1 < \text{Me}^2 < \text{Me}^3 < \text{Me}^4$ (b) $\text{Me}^3 < \text{Me}^4 < \text{Me}^1 < \text{Me}^2$
 (c) $\text{Me}^3 < \text{Me}^1 < \text{Me}^4 < \text{Me}^2$ (d) $\text{Me}^2 < \text{Me}^4 < \text{Me}^3 < \text{Me}^1$
55. The ^1H NMR spectrum of a compound with molecular formula $\text{C}_3\text{H}_7\text{NO}$ shows the following features:
- | | | | |
|----------------------|---------------|---------|---------|
| Chemical shift (ppm) | 6.50 | 2.25 | 1.10 |
| Shape | broad singlet | quartet | triplet |
- Which of the following is in agreement with this information:
- (a) $(\text{CH}_3)_2\text{C} = \text{NOH}$ (b) $\text{CH}_3\text{COCH}_2\text{NH}_2$ (c) $\text{CH}_3\text{CH}_2\text{CONH}_2$ (d) $\text{HCON}(\text{CH}_3)_2$
56. The two fine-structure components of a nuclear magnetic resonance transition are observed at chemical shifts of 2.142 and 2.208 ppm in a 300 MHz NMR spectrometer. Calculate the coupling constant:
- (a) 19.8 Hz (b) 0.066 Hz (c) 6.6 Hz (d) data is insufficient
57. A $\text{C}_5\text{H}_{12}\text{O}_2$ compound has strong infrared absorption at 3300 to 3400 cm^{-1} . The ^1H NMR spectrum has three singlets at δ 0.9, δ 3.45 and δ 3.2 ppm with relative areas 3:2:1. Addition of D_2O to the sample eliminates the lower field signal. The ^{13}C NMR spectrum shows three signals all at higher field than δ 100 ppm. Which of the following compounds best fits this data:
- (a) 1, 5-pentanediol (b) 1, 3-dimethoxypropane
 (c) 2, 2-dimethyl-1, 3-propanediol (d) 2, 4-pentanediol
58. The ^1H NMR spectrum of a compound A shows a doublet and a septet. Which one of the following statements is true:
- (a) The spectrum is consistent with A containing $\text{CH}_3\text{CH}_2\text{CH}_2$ group.
 (b) The spectrum is consistent with A being $(\text{CH}_3)_2\text{CHCl}$.
 (c) The spectrum is consistent with A containing a CH_3CH_2 group.
 (d) The spectrum is consistent with A being $(\text{CH}_3)_2\text{CCl}_2$.
59. A compound of formula C_5H_{12} gives one signal in the ^1H NMR and two signals in the ^{13}C NMR spectra. The compound is:
- (a) Pentane (b) 2-methylbutane
 (c) 2, 2-dimethylpropane (d) Cannot tell without more information
60. The most appropriate spectroscopy for the identification of a nitrile group is:
- (a) IR (b) ^1H NMR (c) UV (d) ESR

61. Compound I gives a strong infrared absorption at 1730 cm^{-1} . ^1H NMR spectrum indicates that it has two types of hydrogen atoms; one H atom appearing as singlet at $\delta = 9.7\text{ ppm}$ and 9H atoms appearing as a singlet at $\delta = 1.2\text{ ppm}$. The structure of I is:



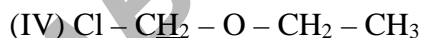
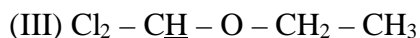
62. The functionality that shows a typical characteristic peak at 2250 cm^{-1} in IR is:



63. Consider a ^1H NMR spectrum in which a quartet and a doublet appeared at 9.72 and 2.40 ppm, respectively. Which of the following compounds is the most probable one:



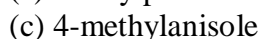
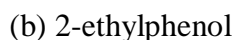
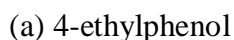
64. The order of decreasing chemical shift in ^1H NMR for the underlined hydrogens is:



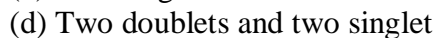
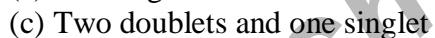
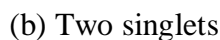
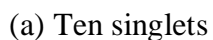
65. The number of normal modes of vibration in the benzene molecule is:



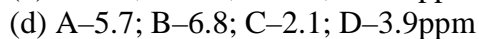
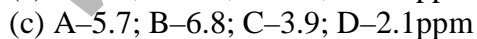
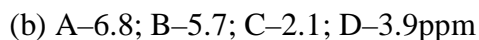
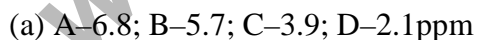
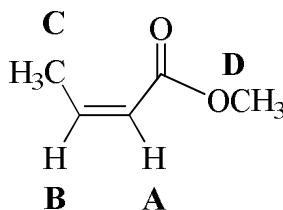
66. An organic compound (MF: $\text{C}_8\text{H}_{10}\text{O}$) exhibited the following ^1H NMR spectral data: δ 2.5 (3 H, s), 3.8 (3H, s), 6.8 (2 H, d, J 8 Hz), 7.2 (2 H, d, J 8 Hz) ppm. The compound among the choices is:



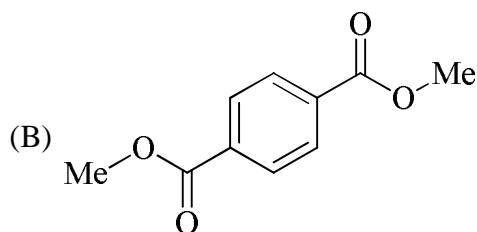
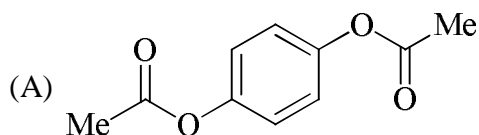
67. The ^1H NMR spectrum of 1, 4-dimethoxybenzene will have:



68. Appropriate ^1H NMR chemical shifts (δ) for the protons A-D for the following compound are:

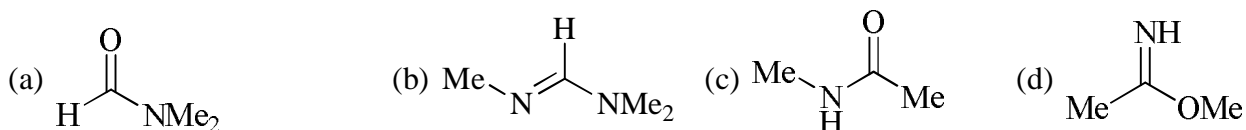


69. Compound A and B exhibit two singlets, each in their ^1H NMR spectra. The expected chemical shifts are at δ :



- (a) 6.9 and 2.1 for A; 7.7 and 3.9 for B
 (b) 7.7 and 3.9 for A; 6.9 and 2.1 for B
 (c) 6.9 and 3.9 for A; 7.7 and 2.1 for B
 (d) 7.7 and 2.1 for A; 6.9 and 3.9 for B

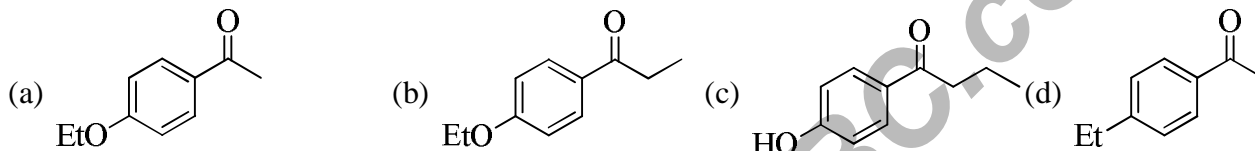
70. In the ^1H NMR spectrum recorded at 293 K, an organic compound ($\text{C}_3\text{H}_7\text{NO}$), exhibited signals at δ 7.8 (1H, s), 2.8 (3H, s) and 2.6 (3H, s). The compound is:



71. An organic compound exhibited the following ^1H NMR spectra data:

δ 7.80 (2 H, d, $J = 8$ Hz), 6.80 (2 H, d, $J = 8$ Hz), 4.10 (2 H, q, $J = 7.2$ Hz),
 2.4 (3H, s), 1.25 (3 H, t, $J = 7.2$ Hz)

The compound, among the choices given below is,



72. In NMR spectroscopy the product the nuclear 'g' factor (g_N), the nuclear magneton (β_N) and the magnetic field strength (B_0) gives the:

- (a) Energy of transition from α to β state
 (b) Chemical shift
 (c) Spin-Spin coupling constant
 (d) Magnetogyric ratio

73. Among the isomers of C_4H_6 given below, the compound which exhibits an absorption band at 3300 cm^{-1} in the IR spectrum, is:

- (a) 1, 3-butadiene (b) 1-butyne (c) 2-butyne (d) cyclobutane.

74. Which of the following absorptions is shown by 1, 3-butadiene in its UV absorption spectrum recorded in n-hexane (ϵ_{max} is the molar absorptivity):

- (a) $\lambda_{\text{max}} 217\text{nm}$ ($\epsilon_{\text{max}} = 21,000$) (b) $\lambda_{\text{max}} 214\text{nm}$ ($\epsilon_{\text{max}} = 210$)
 (c) $\lambda_{\text{max}} 253\text{nm}$ ($\epsilon_{\text{max}} = 50,000$) (d) $\lambda_{\text{max}} 250\text{nm}$ ($\epsilon_{\text{max}} = 500$)

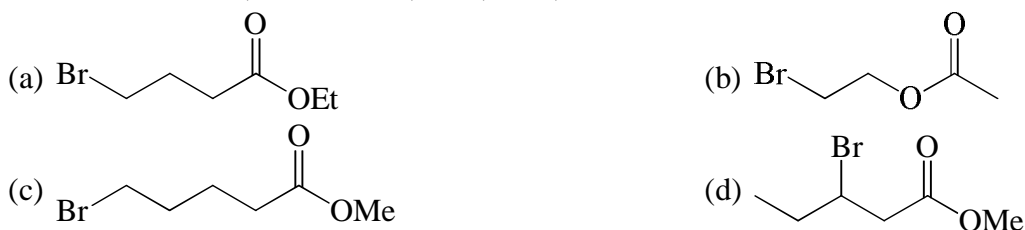
75. Match the observed principal absorptions in the visible spectrum shown in **List-I** with the bond shows this absorption in **List-II**:

- List - I** (1) $\sigma \rightarrow \sigma^*$ (2) $n \rightarrow \sigma^*$ (3) n, π^* (4) π, π^*
List - II (i) C-C (ii) C-O (iii) C=O (iv) C=C
 (a) 1-(i), 2-(ii), 3-(iii), 4-(iv) (b) 1-(i), 2-(iii), 3-(ii), 4-(iv)
 (c) 1-(ii), 2-(i), 3-(vi), 4-(iii) (d) 1-(vi), 2-(ii), 3-(iii), 4-(i)

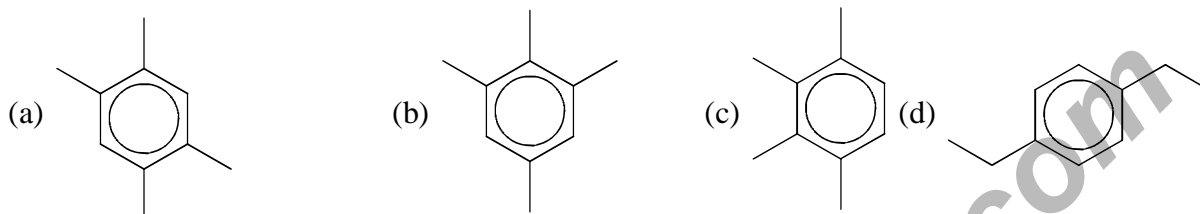
76. The correct structure of the compound based on the following characteristic spectral data is IR: 1736 cm^{-1}

^1H NMR: δ 3.59 (s, 3H), 3.32 (t, 2H), 2.25 (t, 2H), 1.85-1.75 (m, 2H), 1.73-1.62 (m, 2H)

^{13}C NMR: δ 174.0, 51.0, 32.9, 32.8, 31.0, 23.0



77. In atomic absorption spectroscopy, the atomization process utilizes:
 (a) Flame (b) Electric field (c) Magnetic field (d) Electron beam
78. The absorption at λ_{\max} 279 nm in the UV spectrum of acetone is due to:
 (a) $\pi - \pi^*$ transition (b) $n - \pi^*$ transition (c) $\sigma - \sigma^*$ transition (d) $\pi - \sigma^*$ transition
79. An organic compound having the molecular formula $C_{10}H_{14}$ exhibited two singlets in the 1H NMR spectrum and three signals in the ^{13}C NMR spectrum. The compound is:



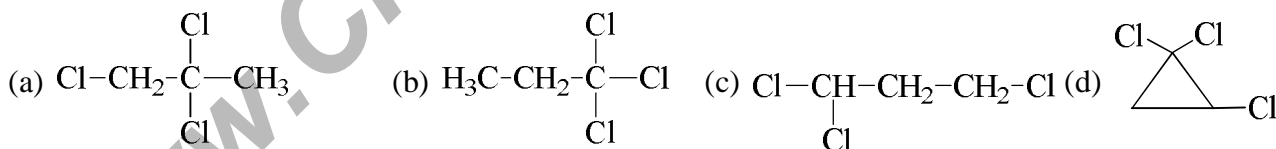
80. A compound with molecular formula $C_5H_{10}O$, exhibit following 1H NMR spectral data - δ 0.95 (6H, d), δ 2.10 (3H, S), δ 2.43 (1H, m). The structure is:



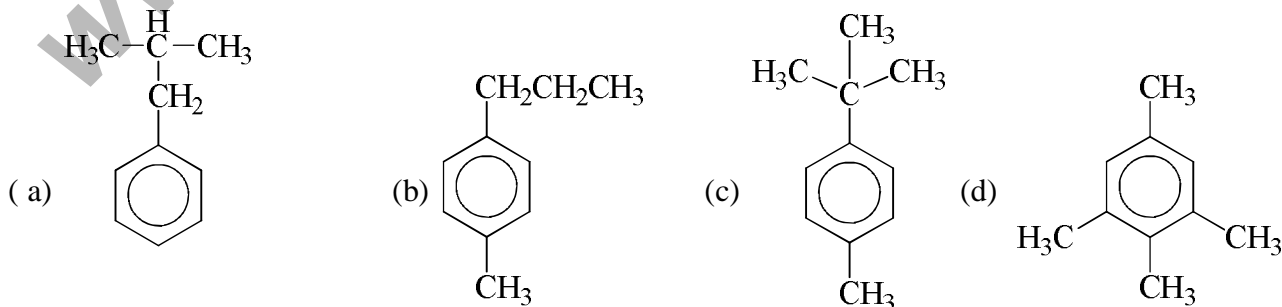
81. A compound with molecular formula C_4H_7BrO exhibit following 1H NMR spectral data - δ 2.11 (3H, S), 3.52 (2H, t, J=6), δ 4.40 (2H, t, J=6). The structure is:



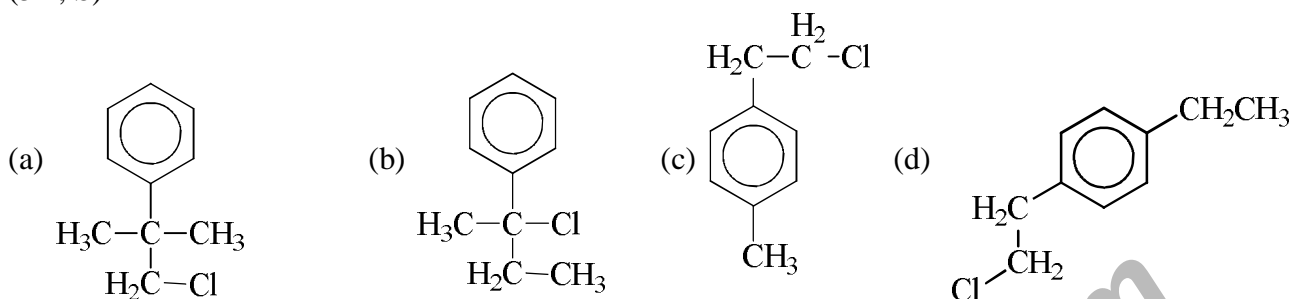
82. A compound with molecular formula $C_3H_5Cl_3$ exhibit following 1H NMR spectral data - δ 2.20 (3H, S), δ 4.02 (2H, S). The structure of the compound is:



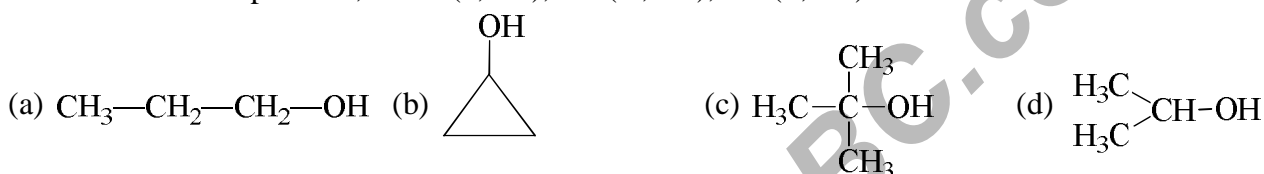
83. A compound with molecular formula $C_{10}H_{14}$ 1H NMR data is δ 1.30 (9H, S), δ 7.28 (5H, S). The structure is:



84. A compound $C_{10}H_{13}Cl$ gave the following 1H NMR data - δ 1.57 (S, 6H), δ 3.07 (2H, S), δ 7.27 (5H, S)



85. A compound has molecular formula C_3H_8O . Its IR spectrum shows a strong absorption band at 3380 cm^{-1} . In 1H NMR spectrum, δ 1.2 (d, 6H), 3.8 (m, 1H), 4.9 (S, 1H). The structure is:



86. A compound is $C_4H_{10}O$ have 1H NMR spectrum is: δ 1.28 (S, 9H), 1.35 (S, 1H). The structure is:



87. How many 1H NMR signals are found in vinyl chloride:



88. The number of signals that appear in proton decoupled ^{13}C NMR of benzonitrile (C_7H_5N) is:



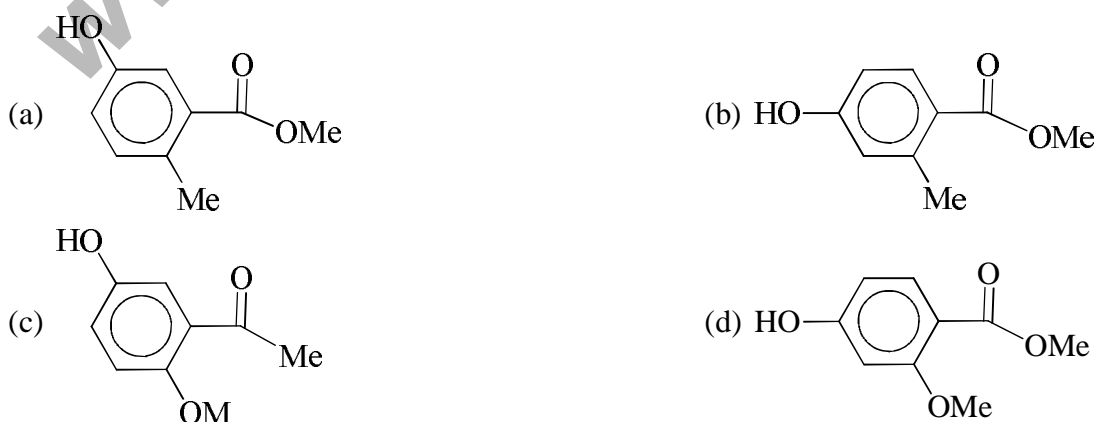
89. The set of proton (bold) in $CH_3CH_2CH_2OCH_3$ that would exhibit different splitting pattern in high (500 MHz) and low (60 MHz) field 1H NMR is:



90. An organic compound ($C_9H_{10}O_3$) exhibit the following spectral data:

IR : $3400, 1680\text{ cm}^{-1}$

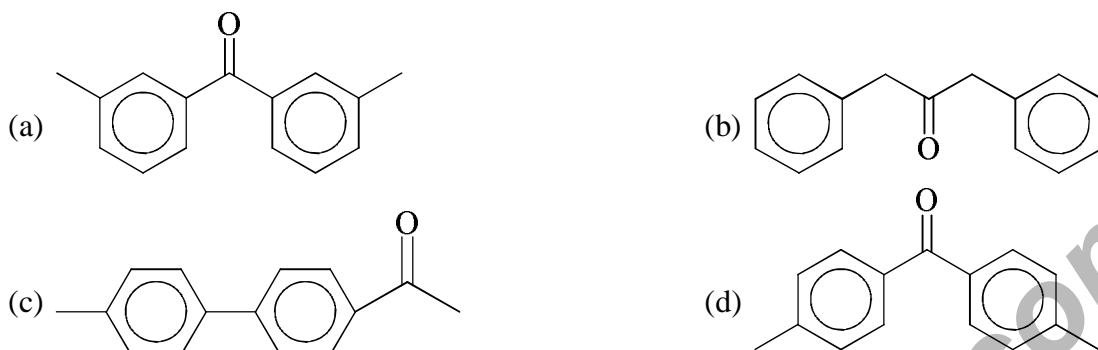
1H NMR : δ 7.8 (1H, d, $J=8\text{ Hz}$), 7.0 (1H, d, $J=8\text{ Hz}$), 6.5 (1H, S), 5.8 (1H, S, D_2O exchangeable), 3.9 (3H, S), 2.3 (3H, S). The compound is:



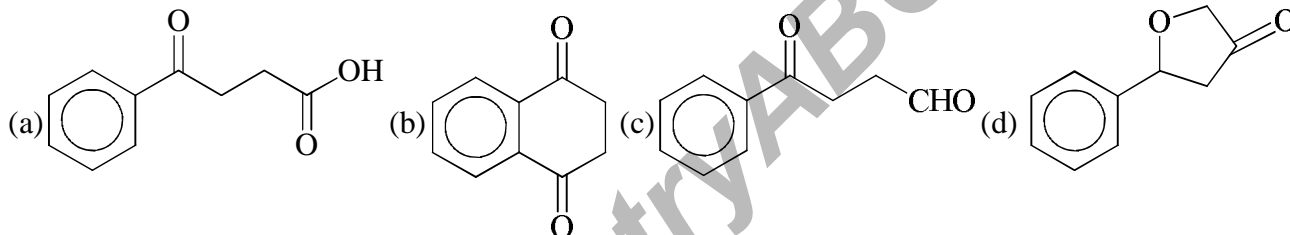
91. An organic compound having molecular formula $C_{15}H_{14}O$ exhibited the following 1H and ^{13}C NMR spectral data:

1H NMR - δ 2.4 (S), 7.2 (d, $J=8Hz$), 7.7 (d, $J=8Hz$)

^{13}C NMR - δ 21.0, 129.0, 130.0, 136.0, 141.0, 190.0



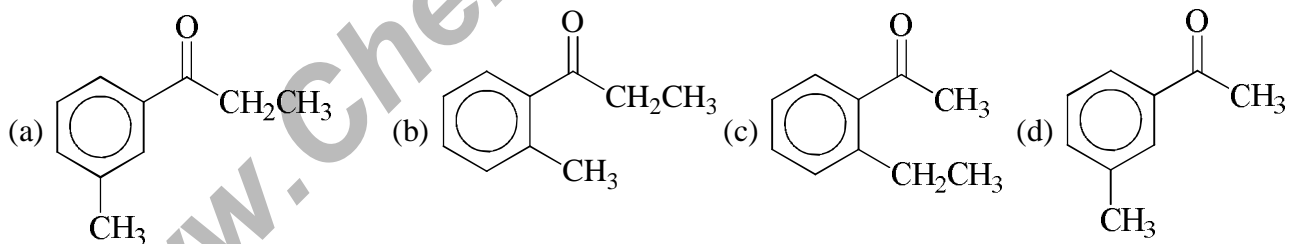
92. The major product compound X formed in the following reaction exhibited a strong absorption at ν_{max} 1765 cm^{-1} in the IR spectrum. The structure of X is:



93. The structure of compound having following characteristic data is:

IR : 1690 cm^{-1}

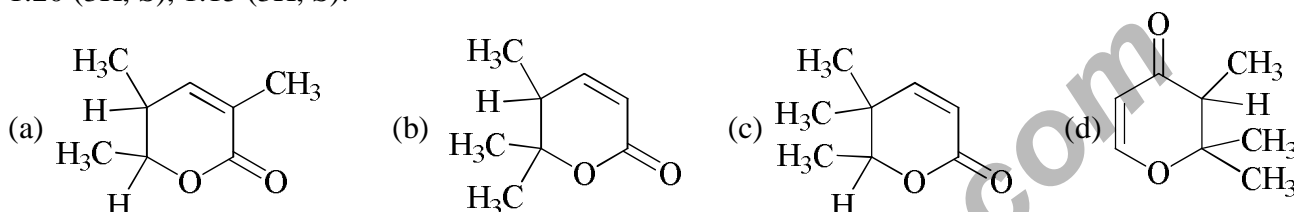
1H NMR - 1.30 (3H, t, $J=7.2$), 2.41 (2H, q, $J=7.2$), 2.32 (3H, S), 7.44 (1H, t, $J=7.0Hz$), 7.57 (1H, dt, $J=7.0, 3.0Hz$), 7.77 (1H, t, $J=3.0Hz$), 7.90 (1H, dt, $J=7.0, 3.0$)



94. The Beckmann rearrangement of a bromo-acetophenone oxime (C_8H_8BrNO) gives a major product having the following 1H NMR - 9.85 (S, 1H), 7.88 (S, 1H), 7.45 (d, 1H, $J=7.2$), 7.17 (m, 1H, 7.12 (d, 1H, $J=7.0\text{ Hz}$), 2.06 (S, 3H). The structure of the product is:



95. ^1H NMR spectrum of [18]-annulene shows:
- (a) Only one peak at δ 7.2 (18 H) (b) Only one peak at δ 5.0 (18 H)
 (c) Two peaks at δ 9.0 (12 H) and δ -3.0 (6H) (d) Two peaks at δ 9.0 (6 H) and δ -3.0 (12 H)
96. In organic compound having molecular formula $\text{C}_8\text{H}_{12}\text{O}_2$ exhibit the following peak in IR and ^1H NMR spectra:
 IR – 1720 cm^{-1}
 ^1H NMR – 6.95 (1H, d, $J=8.5\text{Hz}$), 5.90 (1H, d, $J=8.5\text{Hz}$), 4.53 (1H, q, $J=6\text{Hz}$), 1.41 (3H, d, $J=6\text{Hz}$), 1.20 (3H, s), 1.15 (3H, s):



97. The correct structure of the compound based on the following characteristic spectral data is IR: 1736 cm^{-1} :
- (a) ^1H NMR: δ 3.59 (s, 3H), 3.32 (t, 2H), 2.25 (t, 2H), 1.85-1.75 (m, 2H), 1.73-1.62 (m, 2H) ^{13}C NMR: δ 174.0, 51.0, 32.9, 32.8, 31.0, 23.0



98. For certain magnetic field strength, a free proton spin transition occurs at 700 MHz. Keeping the magnetic field strength constant the ^{14}N nucleus will resonate at ($g(\text{p}) \approx 5.6$ and $g(^{14}\text{N}) \approx 0.4$)
- (a) 700 MHz (b) 400 MHz (c) 200 MHz (d) 50 MHz
99. Predict the multiplicities for hydrogens on C1, C3 and C4 of butanone associated with the spin-spin coupling in its ^1H NMR spectrum:
- (a) H's on C1: Singlet; H's on C3: Doublet; H's on C4: Triplet
 (b) H's on C1: Singlet; H's on C3: Triplet; H's on C4: Quartet
 (c) H's on C1: Singlet; H's on C3: Quartet; H's on C4: Triplet
 (d) H's on C1: Triplet; H's on C3: Doublet; H's on C4: Triplet
100. An organic compound has the following spectroscopic properties: Mass spectrometry: m/z 102 (very small), 87 and 43 are the largest ions; ^1H NMR: δ 1.4 and 3.9 ppm (both singlets, intensity ratio 3:2); ^{13}C NMR: δ 108, 64 and 25 ppm; Infrared spectroscopy: several strong absorptions in the 1000 to 1300 cm^{-1} region. Which of the following is the most likely formula of this compound:



Answer Key

1. d	2. a	3. d	4. b	5. d	6. b	7. b	8. d	9. c	10. a
11. d	12. a	13. c	14. c	15. c	16. d	17. c	18. c	19. a	20. c
21. c	22.	23. a	24. a	25. c	26. c	27. a	28. c	29. c	30. a
31. c	32. c	33. a	34. d	35. c	36. d	37. d	38. b	39. d	40. b
41. c	42. a	43. b	44. c	45. c	46. a	47. a	48. b	49. c	50. a
51. b	52. b	53. a	54. b	55. c	56. a	57. c	58. b	59. c	60. a
61. c	62. d	63. c	64. d	65. b	66. c	67. b	68. d	69. a	70. a
71. a	72. a	73. b	74. a	75. a	76. c	77. a	78. b	79. a	80. a
81. b	82. a	83. c	84. a	85. d	86. b	87. b	88. b	89. b	90. d
91. d	92. d	93. a	94. a	95. c	96. d	97. c	98. d	99. c	100. a