# ALCHEMIST SCIENCE ACADEMY

# Assignments

With Previous Years Questions CSIR-NET Dec 2018 , TIFR- 2018 & GATE 2019

# Spectroscopy

for

CSIR NET/JRF, GATE, TIFR, JNU, Ph.D

# ASSIGNMENT

## Spectroscopy

**ALCHEMIST SCIENCE ACADEMY**

**Website: www.csirnetalchemist.com**
**E-mail: alchemistscienceacademy@gmail.com**
**Head Office: 28-A Jia Sarai, Hauz Khas New Delhi – 16**
**Ph. 011-26511021, 8285787633, 9582285416, 9953942156**

# Contents

## Spectroscopy (M-B, ESR, PES, UV)
## NET Previous Year's Question

Q1. Which of the following spectroscopic techniques will be useful to distinguish between M - SCN and M – NCS binding modes? **[NET June 2011]**

(a) NMR (b) IR (c) EPR (d) Mass

Q2. The Stark splitting for a given field is larger for a molecule AX as compared to BX. Which one of the following is true? ( $\mu$ is the dipole moment) **[NET June 2011]**

(a) $\mu_{AX} = \mu_{BX}$ (b) $\mu_{AX} > \mu_{BX}$ (c) $\mu_{AX} < \mu_{BX}$ (d) $\mu_{BX} = 2\mu_{AX}$

Q3. A molecule, AX has a vibrational energy of 100 $cm^{-1}$ and rotational energy of $10cm^{-1}$. Another molecule BX, has a vibrational energy of 400 $cm^{-1}$ and rotational energy of $40cm^{-1}$. Which one of the following statements about the coupling of vibrational and rotational motion is true **[NET June 2011]**

(a) The coupling is stronger in BX

(b) The coupling is stronger in AX.

(c) Magnitude of coupling is same in both AX and BX

(d) There is no coupling in both AX and BX

Q4. The order of carbonyl stretching frequency in the IR spectra of ketone, amide anhydride is: **[NET June 2011]**

(a) Anhydride > amide > Ketone (b) Ketone > amide > anhydride

(c) Amide > anhydride > ketone (d) Anhydride > Ketone > amide

Q5. The absorption at $\lambda_{max}$ 279nm ($\varepsilon = 15$) in the UV spectrum of acetone is due to **[NET June 2011]**

(a) $\pi - \pi^*$ transition (b) $n - \pi^*$ transition

(c) $\sigma - \sigma^*$ transition (d) $\pi - \sigma^*$ transition

Q6. In the EPR spectrum of tetragonal Cu(II) complex, when $g\|g1 > g_e$ the unpaired electron resides in the orbital. **[NET June 2011]**

(a) $d_{xy}$ (b) $d_{x^2-y^2}$ (c) $d_{z^2}$ (d) $d_{xz}$

Q7. Consider the Compounds, **[NET June 2011]**

(A) $SnF_4$ (B) $SnCl_4$ and (C) $R_3SnCl$

The nuclear quadrupole splitting are observed for

(a) (A),(B) and (C) (b) (A) and (B) only (c) (B) and (C) only (d) (A) and (C) on;y

Q8. The correct value of isomer shift (in Mossbauer spectra) and its exaplanation for Fe(II) – TPP and Fe(III) - TPP respectively from the following are: **[NET June 2011]**

( TPP = tetraphenylporphyrinate)

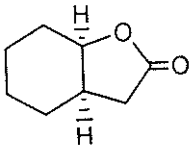
(A) $0.52 mms^{-1}$ (B) $0.45 mms^{-1}$

(C)Increase in s electron density (D) Decrease in s electron density

(a) (A) and (D); (B) and (C) (b) (A) and (C); (B) and (C)

(c)(B)and (D); (A) and (D) (d) (B) and (D); (A) and (C)

Q9. In the IR spectrum, carbonyl absorption band for the following compound appears at **[NET Dec. 2011]**



(a) $1810 cm^{-1}$ (b) $1770 cm^{-1}$ (c) $1730 cm^{-1}$ (d) $1690 cm^{-1}$

Q10. In ${}^{57}Fe'$ Mossbauer experiment source of 14.4 keV (equivalent to $3.48 \times 10^{12} MHz$ ) is moved towards absorber at a velocity of $2.2 mms^{-1}$. The shift in frequency of the source for this sample is **[NET Dec. 2011]**

(a) 35.5 MHz (b)25.5MHz (c) 20.2MHz (d) 15.5MHz

Q11. If Mossbauer spectrum of $Fe(CO)_5$ is recorded in the presence of a magnetic field, the original spectrum with two lines changes into the one with **[NET June 2012]**

(a) Three lines (b) Four lines (c) Five lines (d) Six lines

Q12. The total numbers of fine and hyperfine EPR lines expected for octahedral high spin Mn(II) Complexes are respectively (I = 5/2 for Mn) **[NET June 2012]**

(a) 3 and 30 (b) 5 and 33 (c) 5 and 30 (d) 4 and 24

Q13. The number of lines exhibited by a high resolution EPR spectrum of the species, **[NET Dec. 2012]**

[Cu(ethylenediamine)2]2 + is [Nuclearspin (I) of Cu = 3/2 and that of N = 1]

(a) 12 (b) 15 (c) 20 (d) 36

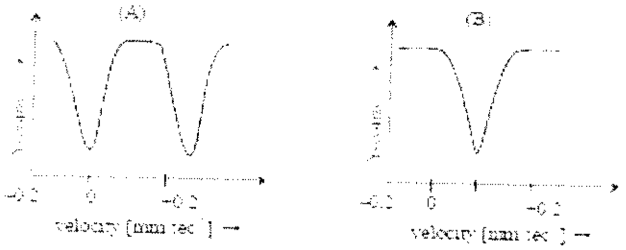
Q14. In the IR spectrum of p-nitrophenyl acetate, the carbonyl absorption band appears at **[NET Dec. 2012]**

(a) 1670 $cm^{-1}$ (b) 1700 $cm^{-1}$ (c) 1730 $cm^{-1}$ (d) 1760 $cm^{-1}$

Q15. The recoil energy of a Massabauer nuclide of mass 139 amu is 2.5MeV. The energy emitted by the nucleus in KeV is **[NET Dec. 2012]**

(a) 12.5 (b) 15.0 (c) 2.05 (d) 25.0

Q16. The Mossbuar spectra of two iron complexes are shown below. They may arise from (i) high-spin iron(III), (ii) high-spin iron(II) and (iii) low-spin iron(III) The correct matches of spectra (A) and (B) with the iron complexes are **[NET June 2012]**



(a) A with (i) and B with (ii) (b) A with (ii) and B with (i)

(c) A with (iii) and B with (ii) (d) A with (ii) and B with (iii)

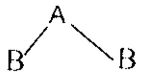
Q17. The number of EPR signals observed for octahedral Ni(II) complexes is **[NET June 2013]**

(a) One (b) Two (c) Three (d) Zero

Q18. A triatomic molecule of the type $AB_2$ shows two IR absorption lines and one IR-Raman line. The structure of the molecule is **[NET June 2013]**

(a) B – B – A (b) B – A – B

(c)


(d)


Q19. In the IR, spectrum, the absorption band due to carbonyl group in phenyl acetate appears at **[NET June 2013]**

(a) 1800 $cm^{-1}$ (b) 1760 $cm^{-1}$ (c) 1710 $cm^{-1}$ (d) 1660 $cm^{-1}$

Q20. Among the following, those can act as Mossbauer nuclei are **[NET June 2013]**

(A) $^{129}I$ (B) $^{57}CO$ (C) $^{57}Fe$ (D) $^{121}Sb$

(a) A, B, C and D (b) B,C and D only

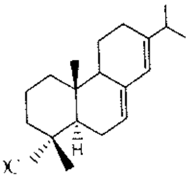
(c) A,B and D only (d) A,C and D only

Q21. For a tetragonally distorted Cr(III) complex, zero field splitting results in the following number of Kramers doublets: **[NET June 2013]**

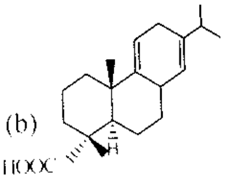
(a) 1 (b) 2 (c) 3 (d) 4

Q22. In the UV-V is spectrum, a diterpenoid exhibited a $\lambda_{max}$ at 275 nm. The compound, among the choice given below is **[NET June 2013]**

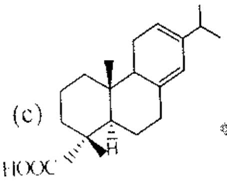
(a)



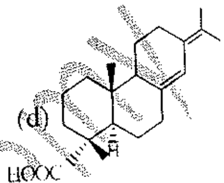
(b)



(c)



(d)



Q23. In the IR spectrum of p-nitrophenyl acetate, the carbonyl absorption band appears at **[NET Dec. 2013]**

(a) 1660 $cm^{-1}$ (b) 1700 $cm^{-1}$ (c) 1730 $cm^{-1}$ (d) 1770 $cm^{-1}$

Q24. In the atomic absorption spectroscopic estimation of Fe(III) using $O_2 / H_2$ flame, the absorbance decreases with the addition of **[NET Dec. 2013]**

(a) $CO_3^{2-}$ (b) $SO_4^{2-}$ (c) EDTA (d) $Cl^{-1}$

Q25. The number of lines in the ESR spectrum of $CD_3$ is (the spin of D is 1) **[NET June 2014]**

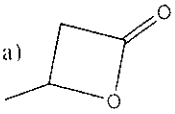
(a) 1 (b) 3 (c) 4 (d) 7

Q26. The correct order of the isomeric shift in Mossbauer spectra ($^{57}$Fe source) of iron compound is **[NET Dec. 2014]**

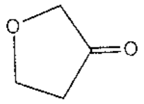
(a) Fe(II > Fe (III) > Fe (IV)
(b) Fe(III) > Fe(II) > FE (IV)
(c) Fe(IV) > Fe (III) > Fe(II)
(d) Fe(IV) > FE(II) > FE (III)

Q27. A compound with molecular formula $C_4H_6O_2$ shows band at 1770 $cm^{-1}$ in IR spectrum and peaks at 178,68,28 and 22 ppm in $^{13}$CNMR spectrum. The correct structure of the compound is **[NET Dec. 2014]**

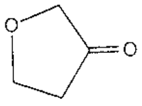
(a)



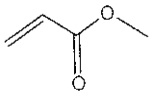
(b)



(c)



(d)



Q28. The gas commonly used in generating plasma in inductively Coupled Plasma Atomic Emission spectroscopy (ICPAES) is **[NET Dec. 2014]**

(a) Argon (b) Carbon dioxide (c) Nitrous oxide (d) hydrogen

Q29. The compound that exhibits sharp bands at 3300 and 2150 $cm^{-1}$ in the IR spectrum is **[NET June 2015]**

(a) 1 - butyne (b) 2 - butyne (c) butyronitrile (d) butylamine

Q30. The reduced form of a metal ion M in a complex is NMR active. On oxidation, the complex gives an EPR signal with $g \approx 2.2$ and $g_{\perp} \approx 2.0$. Mossbauer spectroscopy cannot characteristic the metal complex. The M is **[NET June 2015]**

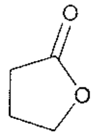
(a) Zn (b) Sn (c) Cu (d) Fe

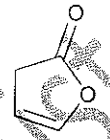
Q31. The resonance Raman stretching frequency $\left(\nu_{0-0}, \text{ in cm}^{-1}\right)$ of $O_2$ is 1580. The $\nu_{0-0}$ for $O_2$ in bound oxyhemoglobin in close to **[NET Dec. 2015]**

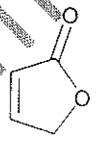
(a) 1600 (b) 1900 (c) 800 (d) 1100

Q32. Correctly matched structure and carbonyl stretching frequency set is **[NET Dec. 2015]**

**Column - A** **Column - B**

(P)  (X)1750cm$^{-1}$

(Q)  (Y)1770cm$^{-1}$

(R)  (Z)1800cm$^{-1}$

(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

Q33. Pick the correct statements about Atomic Absorption Spectrometry (AAS) from the following

**[NET Dec. 2015]**

(A) Hg lamp is not a suitable source for AAS
(B) Graphite furnace is the best atomizer for AAS
(C) Non-metals cannot be determined with AAS
(D) AAS is better than ICP-AES for simultaneous determination of metal ions.
Correct answer is

(a) A,B and C (b) B,C and D (c) A,B and D (d) B and D

Q34. Mossbauer spectrum of a metal complex gives information about **[NET Dec. 2015]**

(A) oxidation state and spin state of metal

(B) types of lingands coordinated to metal

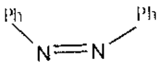
(C) nuclear spin state of metal

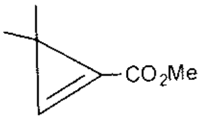
(d) geometry of metal

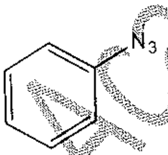
Correct answer is

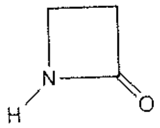
(a) A and C (b) B and C (c) A, B and D (d) B and D

Q35. Among the following, the compound that displays an IR band at 2150 $cm^{-1}$ is **[NET June 2016]**

(a)


(b)


(c)


(d)


Q36. In the UV-visible absorption spectrum of an $\alpha-\beta-$ unsaturated carbonyl compound, with increasing solvent polarity, **[NET June 2016]**

(a) $n-\pi^*$ transitions undergo hypsochromic shift, $\pi-\pi*$ undergo bathochromic shift

(b) $n-\pi^*$ transitions undergo bathochromic shift, $\pi-\pi^*$ undergo hypsochromic shift

(c) both $n-\pi^*$ and $\pi-\pi$ transition undergo bathochromic shift

(d) both $n-\pi^*$ and $\pi-\pi^*$ transitions undergo hypsochromic shift.

Q37. Identify correct statements for the EPR spectrum of VO $(\mathrm{acac})_2$ [with square pyramidal geometry at vanadium] at $77\mathrm{K}\left[I\left(^{51}\mathrm{V}\right)=7/2\right]$. **[NET June 2016]**

(A) It has two g values (B) It has $8$ lines only

(C) It has one g value (D) It has two patterns of $8$ lines each.

(a) A and D (b) A and C (c) B and C (d) B and D

Q38. The record Mossbauer spectrum of Fe containing samples, a source, 'X' is used. X after a nuclear transformation (Y) gives $\lambda-$ radiation used in Mossbauer spectroscopy. **[NET June 2016]**

(a) $^{57}\mathrm{Fe},\beta-$ emission (b) $^{57}\mathrm{Co},\beta-$ wmission

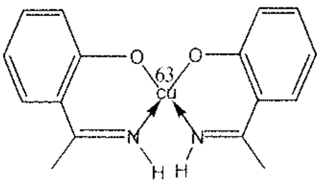
(c) $^{57}\mathrm{Co},\mathrm{e}^-$ capture (d) $^{57}\mathrm{Fe},\mathrm{e}^-$ capture

Q39. The compound which shows IR frequencies both 3314 and 2126 cm$^{-1}$ is **[NET Dec. 2016]**

(a) $CH_3(CH_2)_4CH_2SH$ (b) $CH_3(CH_2)_4CH_2C=N$

(c) $CH_3(CH_2)_4CH_2C=C-H$ (d) $CH_3(CH_2)_2C=C(CH_2)_2CH_3$

Q40. For complex A, deuteration of NH protons does not alter the EPR spectrum. The number of hyperfine line expected in the EPR $\left[I\left({}^{63}Cu\right)=\frac{3}{2}\right]$ spectrum of A is **[NET Dec. 2016]**



(a) 20 (b) 12 (c) 60 (d) 36

Q41. Mossbauer spectrum of complex $\left[Fe(1,10-\text{phenanthroline})_2(NCS)_2\right]$ show two line at 300 K, four lines at 186K and again two lines at 77K. This can be attributed to **[NET June 2017]**

(A) Change in the coordination mode of NCS

(B) Change in the spin-state of iron

(C) cis-trans isomerisation

(D) change in metal-ligand bond distances

The correct statements are

(a) A and B (b) B and C (c) A and C (d) B and D

Q42. $(R_3Ge)_2$ on photolysis gives a radical which shows ESR spectrum. The ESR signals carrying the signature of $^{73}Ge(I=9/2)$ are in terms of **[NET June 2017]**

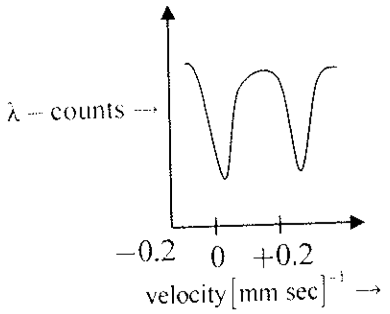
(a) Nine line (b) Tenlines (c) two lines (d) one line

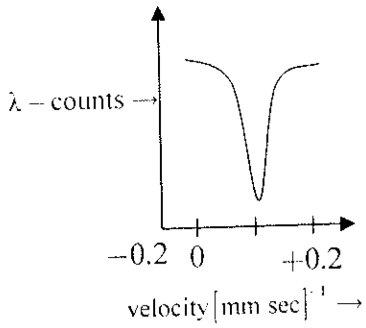
Q43. The resonance Raman stretching frequency (in cm$^{-1}$) of the bound $O_2$ species in oxy-hemerthyrin and oxyhemoglobin, respectively, are **[NET June 2017]**

(a) ~850 and 1100 (b) ~ 750 and 850

(c) ~ 850 and 850 (d) ~ 1100 and 850

Q44. The Mossbaur spectra of two iron complexes are shown below. The may arise from (i) high spin iron(III) (ii) high-spin iron (II) and (iii) low-spin iron(III) **[NET June 2012]**



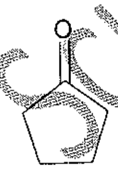
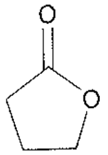
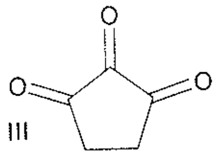


The correct matches of spectra (A) and (B) with the iron complex are

(a) A with (i) and B with (ii)  (b) A with (ii) and B with (i)

(c) A with (iii) and B with (ii)  (d) A with (ii) and B with (iii)

Q45. Correct match of the compounds in column P with the IR stretching frequencies $(cm^{-1})$ in Column Q is **[Net Dec. 2018]**

| **Column P** | **Column Q** |
|---|---|
| I  | A 1865 |
| II  | B 1770 |
| III  | C 1745 |

(a) I – B; II – C; III – A  (b) I – C; II – A; III – B  (c) I – C; II – B; III – A  (d) I – A; II – C; III – B

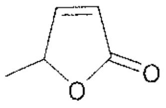
Q46. The number of lines in EPR spectrum of $CD_3\left(I_{D=1}\right)$ **[NET June 2018]**

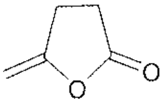
(a) 3  (b) 5  (c) 7  (d) 9

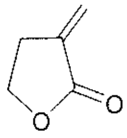
Q47. Consider the species $No, I_2, I_2^-, Cu^{2+}$ and $VO^{2+}$. The number of paramagnetic species among them and the EPR inactive species, respectively, are

(a) 4 an $I_2^-$ (b) 4 and $I_2$ (c) 3 and $VO^{2+}, Cu^{2+}$ (d) 3 and NO, $Cu^{2+}$

Q48. In IR spectra the stretching frequency $\left(\text{in cm}^{-1}\right)$ of the carbonyl group of the following compounds is in the order **[NET Dec. 2018]**


**(A)**


**(B)**


**(C)**

(a) B > A > C (b) A > C > B (c) B > C > A (d) C > B > A

Q49. Arrange the following molecules in order of increasing fundamental frequencies **[NET Dec. 2018]**

(a) $O_2^{2-} < O_2^{-} < O_2 < O_2^{+}$ (b) $O_2 < O_2^{+} < O_2^{-} < O_2^{2-}$

(c) $O_2^{2-} < O_2 < O_2^{-} < O_2$ (d) $O_2^{+} < O_2 < O_2^{-} < O_2^{2-}$

## Answer Key

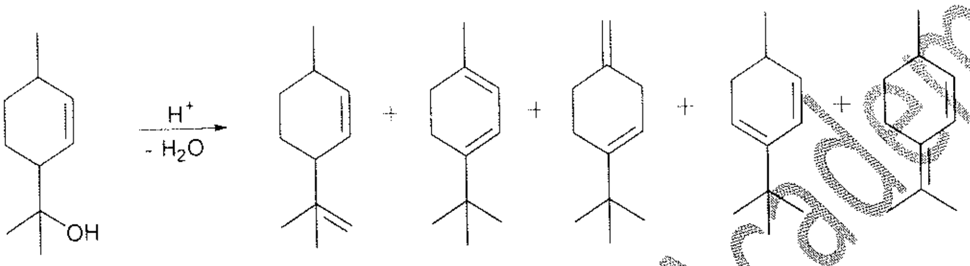
| | | | | | | |
|---|---|---|---|---|---|---|
| Q1.(b) | 2.(b) | 3.(a) | 4.(d) | 5.(c) | 6.(b) | 7.(d) |
| 8.(a) | 9.(b) | 10.(b) | 11.(d) | 12.(c) | 13.(d) | 14.(d) |
| 15.(d) | 16.(a) | 17.(b) | 18.(b) | 19.(d) | 20.(b) | 21.(c) |
| 22.(d) | 23.(b) | 24.(d) | 25.(a) | 26.(a) | 27.(c) | 28.(a) |
| 29.(a) | 30.(c) | 31.(d) | 32.(a) | 33.(a) | 34.(d) | 35.(c) |
| 36.(a) | 37.(c) | 38.(c) | 39.(c) | 40.(a) | 41.(d) | 42.(b) |
| 43.(d) | 44.(b) | 45.(c) | 46.(c) | 47.(b) | 48.(c) | 49(a) |

## GATE Previous Year's Question

Q1. Among the isomers of $C_4H_6$ given below, the compound which exhibits an babsorption band at 3300cm $^{-1}$ in the IR spectrum, is **[GATE 2002]**

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

Q2.



On the basis of Woodward-Fieser rules, the dienes that have $\lambda_{max}$ values in the range 268 – 273nm are **[GATE 2003]**

(a) P and Q (b) P and R (c) Q and R (d) Q and S

Q3. The number of hyperfine split lines observed in ESR spectrum of methyl radical is **[GATE 2004]**

(a) 1 (b) 4 (c) 6 (d) 8

Q4. Match the compounds P – S with their carbonyl stretching frequency $(cm^{-1})$ I – VI in IR spectroscopy. **[GATE 2004]**

| | |
|---|---|
| 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

Q5. Out of the following, the one which is not an excitation source for IR spectrometers is **[GATE 2005]**

(a) tungaten filament lamp (b) Nernst glower

(c) deuterium lamp (d) mercury are

Q6. The moleculer active in rotational microwave, infrared absorption as well as rotational Raman spectra is **[GATE 2006]**

(a) $CO_2$ (b) $SF_6$ (c) HCl (d) $H_2$

Q7. A radical contains $^{14}N\left(I=1\right)$ with hyperfine constant 1.61mT and Two equivalent protons (I = 1/2) with hyperfine constant 0.35mT. The ESR spectrum will exhibit. **[GATE 2006]**

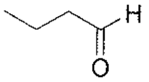
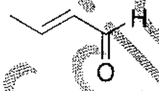
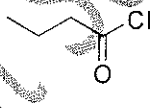
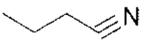
(a) 3 line (b) 6 line (c) 7 line (d) 9 line

Q8. Which of the following absorptions is shown by 1,3 - butadiene in its UV absorption spectrum recorded in n-hexane ( $\varepsilon_{max}$ is the molar absorptivity )? **[GATE 2006]**

(a) $\lambda_{max}\,217nm\left(\varepsilon_{max}=21,000\right)$ (b) $\lambda_{max}\,214nm\left(\varepsilon_{max}=210\right)$

(c) $\lambda_{max}\,253nm\left(\varepsilon_{max}=50,000\right)$ (d) $\lambda_{max}\,250nm\left(\varepsilon_{max}=500\right)$

Q9. Match of the compounds in **list-I** with the stretching frequencies $\left(cm^{-1}\right)$ of the principle function groups given in **List-II** **[GATE 2006]**

| | |
|---|---|
| (1)  | (i) 2240 |
| (2)  | (ii) 1795 |
| (3)  | (iii) 1750 |
| (4)  | (iv) 1750 |
| | (v) 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

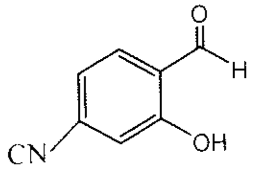
Q10. Match the observed principle absorptions in the visible spectrum shown in **List-I** With the bond shows this absorption in **list-II** **[GATE 2007]**

| **List-I** | **List-II** |
|---|---|
| (1) $\sigma\rightarrow\sigma^*$ | (i) C – C |
| (2) $n\rightarrow\sigma^*$ | (ii) C – O |
| (3) $n,\pi^*$ | (iii) C = O |
| (4) $-\pi,-\pi^*$ | (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-(iv), 4-(iii) (d) 1-(iv), 2-(ii), 3-(iii), 4-(i)

Q11. The IR stretching frequencies $(cm^{-1})$ for the compound X are as follows:3300 – 3500 (s,br);3000(m); 2225(s);1680(s) **[GATE 2008]**



The correct assignment of the absorption band is

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

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

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

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

Q12. The total number of ways in which two nonidentical spin 1/2 particles can be oriented relative to a constant magnetic fields is; **[GATE 2008]**

(a) 1 (b) 2 (c) 3 (d) 4

Q13. The Oxidation sate of the metal ion in the catalyst can be deducted by **[GATE 2008]**

(a) Atomic absorption spectroscopy (b)Mossbauer spectroscopy

(c) HPLC (d) Gas Chromatography

**Common data for Q .15 and Q. 16**

A six –coordinate transition-metal complex is ESR and Mossbauer active. The effective magnetic moment of this complex is ~ 5.9 B.M.

Q14. The metal ion along with its oxidation state and the number of unpaired electron present are**[GATE 2010]**

(a) Fe(II) and 4 (b) Mn(II) and 5

(c) Fe(III) and 1 (d) Fe(III) and 5

Q15. The complex is **[GATE 2010]**

(a) $\left[Mn(H_2O)_6\right]^{2+}$ (b) $\left[Fe(CN)_6\right]^{3-}$

(c) $\left[Fe(H_2O)_6\right]^{2+}$ (d) $\left[Fe(H_2O)_6\right]^{3+}$

Q16. The extent of Mossbauer quadrupole splitting of iron follows the order **[GATE 2012]**

(a) $FeCl_2 4H_2O > k_2[Fe(CN)_5(NO)] > FeCl_3 6H_2O$

(b) $K_2[Fe(CN)_5(NO)] > FeCl_2.4H_2O > FeCl_3.6H_2O$

(c) $FeCl_3.6H_2O > K_2[Fe(CN)_5(NO)] > FeCl_2.4H_2O$

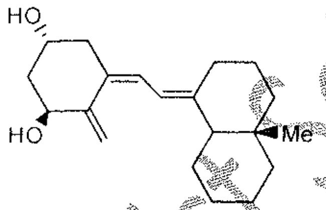
(d) $FeCl_2.4H_2O > FeCl_3.6H_2O > K_2[Fe(CN)_5(NO)]$

Q17. 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 **[GATE 2014]**

(a) 1,2 - butadiene (b) 1, 3 – butadiene

(c) 1 - butyne (d) 2- butyne

Q18. Given the fact $1,3-$ butadiene has a UV absorption of 217 nm, the absorption wavelength ( in nm) for the conjugated system shown below is **[GATE 2014]**



(Use these absorption values for auxochromic groups:

Alkyl: + 5 exo-cyclic double bond + 5 every additional conjugated C = C 30)

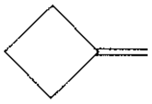
Q19. In atomic absorption spectroscopy, the atomization process utilizes **[GATE 2014]**

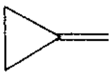
(a) flame (b) electric field

(c) magnetic field (d) electron beam

Q20. The correct order of IR stretching frequency of the $C = C$ in the following olefins is **[GATE 2014]**


I


II


III

(a) I > II > III (b) II > III > I (c) III > II > I (d)III > I > II

Q21. The value of '$g$' and the number of signal observed for the reference standard diphenylpicrylhydrazyl (DPPH), in the solid state ESR spectrum are, respectively **[GATE 2015]**

(a) 2.0036 and 1 (b) 2.0036 and 3

(c) 2.2416 and 1 (d) 2.2416 and 3

Q22. The $\nu_{0-0}$ resonance resonance Raman stretching frequency (in $\mathrm{cm}^{-1}$) of the $O_2$ coordinated to iron centre in oxyhemoglobin is nearly **[GATE 2017]**

(a) 1100 (b) 850 (c) 1550 (d) 1950

Q23. The characteristic feature of an electron spin resonance (ESR) Spectrum of frozen aqueous solution of $CuSO_4.5H_2O$ at 77 k is **[GATE 2017]**

(a) $g_{\parallel} > g_{\perp}$ (b) $g_{\parallel} < g_{\perp}$ (c) $g_{\parallel} = g_{\perp}$ (d) $g_x \neq g_y \neq g_z$

## Answer Key

Q1.(b) 2.(d) 3.(b) 4.(c) 5.(d) 6.(c) 7.(d)
8.(a) 9.(c) 10.(d) 11.(a) 12.(a) 13.(b) 14.(d)
15.(d) 16.(d) 17.(c) 18.(282) 19.(a) 20.(c) 21.(a)
22.(a) 23.(a)

## TIFR Previous Year's Question

Q1. It is not easy to locate H atoms in the structure of proteins obtained by X-ray diffraction due to which of the following reasons: **[TIFR 2010]**

(a) H atoms are transparent to the X-rays

(b) H - bonding interaction present in protein structures

(c) interaction of H with solvent molecules

(d) Very low levels of scattering of X-rays by H

Q2. Arrange the characteristic timescalses of the following set of dynamical spectroscopic techniques in decreasing order of time (longest to shortest); NMR (Nuclear Magnetic Resonance), ESR ( Electron spin Resonance), Fluorescence, Raman and absorption. **[TIFR 2011]**

(a) absorption > NMR > Fluorescence > ESR > Raman

(b) NMR > ESR > Fluorescence > Raman > Absorption

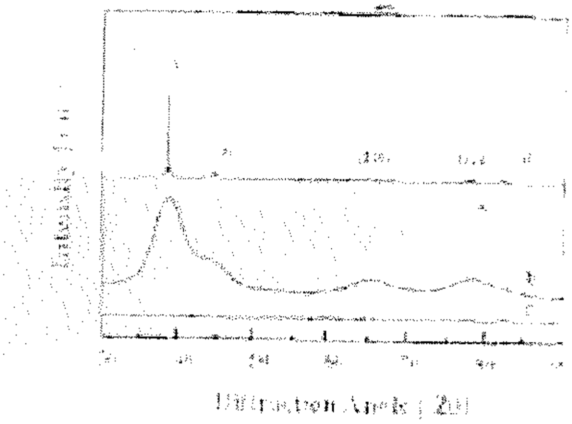
(c) Fluorescence > Absorption > ESR > NMR > Raman

(d) All have similar characteristic timescales.

Q3. In a chemistry lab, the aim of an experiment was to generate well structured, 5 nm sized gold nanoparticles. A student experimented with the following synthesis: **[TIFR 2013]**

I-nonanethiol $\left(C_9H_{19}SH\right)$ and $HAuCl_4$ were first mixed (in a molar ratio of 10 : 1, and then gold ions were reduced by slowly adding $NaBH_4$. In this synthesis after 2 hours no precipitate was observed and only a very faint pink colloidal solution was obtained. This solution was then evaporated onto a glass slide and the sample characterized by X-ray diffraction.

Given below are three XRD patterns. One but of these three patterns was obtained by the student when he / she characterized the sample on the glass slides. Which statement below is true?



(a) The synthesis did not yield gold nanoparticles as there was no precipitate, therefore the XRD pattern that will be obtained is that shown as curve (c) – It is almost a flat baseline indicating no product.

(b) 5 nm gold nanoparticles were formed and XRD pattern shown as (a) represents the product. It signifies that the nanoparticles are crystalline and the face-centered cubic (fcc) crystal structure can be clearly used to index the peaks.

(c) 5nm gold nanoparticles will show size-dependent line broadening and therefore if the product consisted of such particles, then curve (b) will be obtained.

(d) None of the above statements are true.

Q4. 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 mole **[TIFE 2013]**

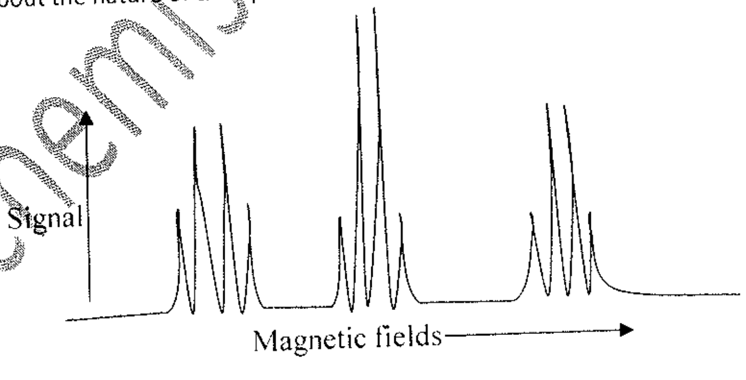
(a) $10^{18} - 10^{-23}, 10^{-13} - 10^{-21}, 10^{13} - 10^{-16}, 10^{-9} - 10^{-11}$

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

Q5. A magnetic resonance spectrum, recorded using a radiation of frequency 100 is shown below. What can you say about the nature of this spectrum ? **[TIFR 2015]**



(a) It is a continuous-wave NMR spectrum

(b) It is fourier transform NMR spectrum

(c) It is an ESR spectrum

(d) None of the above

Q6. A long column of water in any transparent bottle appears slightly blue. However, If we replace water with heavy water $(D_2O)$ it will look more transparent. This effect is due to **[TIFR 2016]**

(a) Rayleigh scattering

(b) Kinetic isotope effects

(c) Absorption spectra of $H_2O$ and $D_2O$ are different

(d) None of the above.

Q7. For electronics transitions in organic molecules, the expected energy ordering the transitions is: **[TIFR 2018]**

(a) $\pi$ to $\pi^*$ n to $\sigma^* < \sigma$ to $\sigma^* <$ n to $\pi^*$ (b) $\pi$ to $\pi^* <$ n to $\pi^* <$ n to $\sigma^* < \sigma$ to $\sigma^*$

(c) n to $\pi^*$ $\pi$ to $\pi^* <$ n to $\sigma^* < \sigma$ to $\sigma^*$ (d) n to $\sigma^* < \sigma$ to $\sigma^* <$ n to $\pi^* < \pi$ to $\pi^*$

## Answer Key

Q1.(*) 2.(*) 3.(c) 4.(a) 5.(c) 6.(c) 7.(c)

## Other Examinations Previous Year's Question

Q1. The two characteristic stretching frequencies $(\mathrm{cm}^{-1})$ observed in the IR spectrum of compounds containing $NO_2$ group is

(a) 3400 and 3300 (b) 1860 and 1760

(c) 1550 and 1350 (d) 2250 and 1760

Q2. The UV-light source used in UV-visible spectrophotometer is

(a) Mercury lamp (b) Tungsten lamp

(c) Deuterium lamp (d) Sodium lamp

Q3. The recoil velocity ( in $\mathrm{ms}^{-1}$ ) of a free Mossbauer nucleus of mass $10^{-25}$ kg while emitting a $\gamma$ - ray of 0.1 nm wavelength is:

(a) 6.626 (b) 66.26 (c) 662.6 (D) 6626

Q4. The number of lines that appear in the EPR spectrum of $[C_6H_6]$ is

(a) 5 (b) 7 (c) 11 (d) 13

Q5. Which of the following molecules will not absorb infrared radiation ?

(a) CO (b) $Cl_2$ (c) $COCl_2$ (d) $CO_2$

Q6. Which of the following molecules will have the highest zero point vibrational energy?

(a) $CF_4$ (b) $CH_4$ (c) $CCl_4$ (d) $CBr_4$

Q7. For $CO_2$ molecule,

(a) All the vibrational modes are either IR or Raman active

(b) The number of IR and Raman active vibrations will be the same

(c) All vibrations are IR active

(d) All vibrations are Raman active.

Q8. The presence of hydrogen bonding in an organic compound can easily be established utilizing the following technique

(a) IR spectroscopy (b) Mass spectra

(c) Cyclic voltametry (d) CD-ORD

Q9. Which of the following will most conveniently confirm if a know solid sample is impure?

(a) NMR (b) Mass spectrum (c) IR spectrum (d) Melting point

Q10. The molecule azulene has an absorption maximum at 700nm, the red and of the visible spectrum. The next shortest wavelength occurs at 357 nm. The predicated color that azulene can exhibit is:

(a) blue (b) red (c) indigo (d) green

Q11. The anti Stokes lines are generally weaker in intensity because, the

(a) molecules absorb the radiation completely

(b) incident radiation is unpolarized

(c) atoms are generally in the ground state:

(d) vibrational energies are small.

Q12. Which of the two compounds will be most readily separated by TLC ( thin layer chromatography)?

(a) naphthalene and anthracene

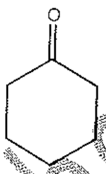
(b) naphthalene and acetophenone

(c) acetophenone and 4- methylacetophenone

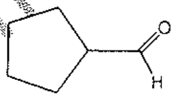
(d) benzoic acid and 3- toluic acid.

Q13. Compound X having molecular formula $C_6H_{10}O$ exhibits absorption at $1700 cm^{-1}$ in the IR spectrum and forms oxime. Compound X yields adipic acid on oxidation. The structure of the compound X is:

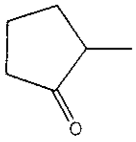
(a)



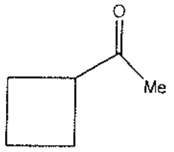
(b)



(c)



(d)



Q14. What is the $\lambda_{max}$ for the following compound? Use the provided parameters for your calculation.

Transoid base value 214nm

Cisoid base value 253nm

Alkyl groups on base + 5nm

Extanded condiation + 30 nm

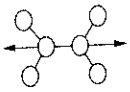
(a) 234nm (b) 244nm (c) 273nm (d) 283nm

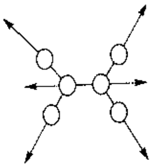
Q15. Of the molecules $CH_4, CO_2$ , benzene and $H_2$ , the ones that will absorb infrared radiation are

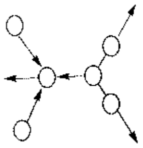
(a) $CH_4, CO_2$ benzene (b) $CH_4$ , benzene and $H_2$

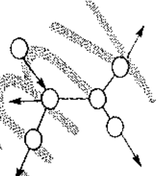
(c) $CO_2$ benzene and $H_2$ (d) $CH_4, CO_2$ and $H_2$

Q16. Which one of the normal modes of ethylene is active in the infared ?

(a)


(b)


(c)


(d)


Q17. The H-H distance in $H_2$ molecule can be determine by,

(a) Microwave rotational spectroscopy (b) Infrared vibrational spectroscopy

(b) NMR spectroscopy (d) Rotational Raman spectroscopy

Q18. The virbrational stretching frequency of $N_2$ can be determined using

(a) Infrared spectroscopy (b) Microwave spectroscopy

(c) Raman spectroscopy (d) NMR spectroscopy

Q19. The number of IR active vibrational modes in ammonia is:

(a) 6 (b) 4 (c) 2 (d) 3

Q20. The molecule that will not have anyabsorbance in the microwave or the infrared region of the electromagnetic spectrum is:

(a) $CO_2$ (b) HF (c) $CH_4$ (d) $H_2$

Q21. The infrared spectrum of $CO_2$ exhibits the following number of absorptions:

(a) One (b) Two (c) Three (d) Four

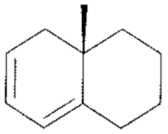
Q22. Which of the following molecules shows EPR resonance?

(a) $H_2O$ (b) $O_2$ (c) $H_2O_2$ (d) $CO_2$

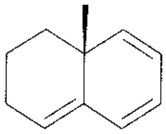
Q23. Which of the following electronics transitions is disallowed?

(a) $\pi \rightarrow \pi^*$ (b) $\sigma \rightarrow \sigma^*$ (c) $n \rightarrow \pi^*$ (d) $\delta \rightarrow \delta^*$

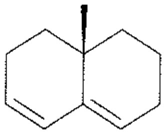
Q24. The order of $\lambda_{max}$ in the UV-Visible spectra for compound. A – C is:



A



B



C

(a) A > B > C (b) B > A > C (c) B > C > A (d) C > B > A

Q25. The number of vibrational degrees of freedom in a gaseous mixture of $^{35}Cl_2O$, $^{37}Cl_2O$ and $^{35}Cl^{37}ClO$ is

(a) 1 (b) 2 (c) 3 (d) 4

Q26. IR stretching frequency of carbonyl group in aldehydes are 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

Q27. The number of peaks in the ESR spectrum of $CH_3$ radical is:

(a) 1 (b) 2 (c) 3 (d) 4

Q28. In the UV spectrum of cyclohexenone, the absorption at $\lambda_{max}$ ~215nm is due to the transition

(a) $\sigma \rightarrow \sigma^*$ (b) $\sigma \rightarrow n$ (c) $\pi \rightarrow n$ (d) $\pi \rightarrow \pi^*$

Q29. The most convenient spectroscopic technique to establish the presence of inter-molecular hydrogen bonding in hydroxy compounds is

(a) UV (b) IR (c) EPR (d) Mass

Q30. Spectrum of a gaseous containing $H_2D_2O_2$ and $N_2$ shows

(a) 4150, 1560, 2200 and 2950 (b) 1560, 2200, 4150 and 2950

(c) 4150, 2950, 1560 and 2200 (d) 2950, 2200, 1560 and 4150

Q31. The source of ultra-violet radiation used in UV-visible Spectrophotometer is

(a) Mercury vapour lamp (b) Sodium vapour lamp

(c) Halogen vapour lamp (d) Hydrogen vapour lamp.

Q32. Among the following, the correct statements is:

(a) Absorption of radiation shifts to longer wavelength region with increase in conjugation

(b) Absorption of radiation shifts to higher energy region with increase in conjugation

(c) Intensity of $n \rightarrow \pi^*$ transition decreases upon conjugation.

(d) Intensity of $\sigma \rightarrow \sigma^*$ transition decreases upon conjugation.

Q33. The infrared and Raman spectrum of $BF_3$ are expected to show:

(a) The same number of peaks

(b) More absorption peaks in IR in comparison to Raman

(c) More absorption peaks in Raman in comparison With IR

(d) Absorption peaks present in Raman are absent in IR

Q34. Among the following diatomic molecules, the one that shows EPR signals is:

(a) $Li_2$ (b) $B_2$ (c) $C_2$ (d) $N_2$

Q35. Which of the following molecules, will have $n \rightarrow \pi^*$ transition at the longest wavelength ?

(a) HCHO (b) $CH_3COC_2H_5$

(c) $C_6H_5COC_6H_5$ (d) $CH_3COC_6H_5$

Q36. The total number of vibrational degrees of freedom of $H_2O_2$ is:

(a) 7 (b) 6 (c) 4 (d) 9

Q37. Resonant frequencies for EPR and NMR are respectively in the spectral region

(a) Microwave and Far-IR (b) Far –IR and microwave

(c) Radiofrequency and microwave (d) Microwave and radiofrequency

Q38. Two samples have been given to you: $\left[NiCl_2(PPh_2)_2\right]$ and $\left[PdCl_2(PPh_3)_2\right]$. A physical method that can be used to identify these compounds unambiguously is

(a) HPLC (b) Magnetic susceptibility

(c) $^{13}C$ NMR spectroscopy (d) Mossbauer spectroscopy

Q39. Which among the following electronic transitions will have the lowest energy.

(a) $n \rightarrow \sigma^*$ (b) $n \rightarrow \pi^*$ (c) $\sigma \rightarrow \sigma^*$ (d) $\pi \rightarrow \pi^*$

Q40. Which of the following molecules shows rotational absorption spectrum?

(a) $CO_2$ (b) OCS (c) $CH_4$ (d) $C_6H_5$

Q41. The H-H distance in $H_2$ molecule can determined by,

(a) Microwave rotational spectroscopy (b) Infrared vibrational spectroscopy

(c) NMR spectroscopy (d) Rotational Raman spectroscopy

Q42. The number of vibrational degrees of freedom in a gaseous mixture of $^{35}Cl_2O$, $^{37}Cl_2O$ and $^{35}Cl^{37}ClO$ is

(a) 1 (b) 2 (c) 3 (d) 4

Q43. Cis and Transe cinnamic acids can be most readily distinguished and identified by,

(a) IR spectra (b) UV spectra

(c) Chemical shift of the olefinic hydrogens (d) Coupling constant of the olefinic hydrogens.

Q44. The region of electromagnetic spectrum employed in the electron spin resonance (ESR) spectroscopy is

(a) radiowave (b) microwave (c) infrared (d) visible

Q45. The number of rotational degrees of freedom of $CO_2$ is

(a) one (b) two (c) three (d) four

Q46. Identify the molecule whose rotational constant can not be determined by spectroscopic methods

(a) $CH_4$ (b) $H_2$ (c) $CO_2$ (d) HCL

Q47. Observe the following statements

I. Atomic mass of isotopes can be obtained from rotational spectra

II. The separation between two successive rotational spectral lines of gaseons NO is $2B\ cm^{-1}$

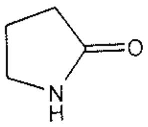
III. The NMR spectrum of a compoundgave a singlet at 300 Hz away from TMS using a NMR spectrometer operating at 60 MHz. Its chemical shift is 3 ppm

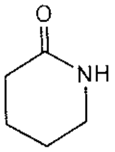
Which of the following is correct?

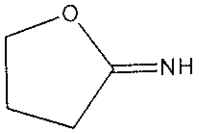
(a) I,II and IIIare correct (b) only III is correct

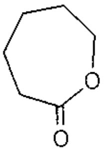
(c) I and II are correct (d) Only I is correct

Q48. Which among the following exhibits a carbonyl absorbtion band at $1770\text{cm}^{-1}$

**(a)**


**(b)**


**(c)**


**(d)**


Q49. Among the following molecules, one having the highest zero point vibrational energy is

(a) HF (b) $CH_4$ (c) $H_2O$ (d) $NH_3$

Q50. The number of hyperfine lines in the EPR spectrum of a one electron reduced product of $\left[Co_3(CO)_9Se\right](I = 7/2 \text{ for Co nucleus})$ is

(a) 8 (b) 15 (c) 22 (d) 1

Q51. Which of the followings species is ESR active?

(a) $VOSO_4$ (b) $K_2Cr_2O_7$ (c) $KMnO_4$ (d) $\left[Co(NH_3)_6\right]Cl$

Q52. Which one of the following exhibits rotational spectra ?

(a) $H_2$ (b) $N_2$ (c) CO (d) $CO_2$

Q53. 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

Q54. An examination of saturated hydrocarbons containing methyl group show asymmetrical $(V_s)$ Stretching modes in the region of

(a) 2960 and 2870 $cm^{-1}$ (b) 3200 and 3100 $cm^{-1}$

(c) 1800 – 1700 $cm^{-1}$ (d) 1650 – 1450 $cm^{-1}$

## Answer Key

1.(c) 2.(c) 3.(b) 4.(b) 5.(b) 6.(b) 7.(a)

8.(a) 9.(d) 10.(d) 11.(c) 12.(b) 13.(a) 14.(d)

15.(a) 16.(c) 17.(d) 18.(c) 19.(a) 20.(d) 21.(c)

22.(b) 23.(c) 24.(b) 25.(c) 26.(c) 27.(b) 28.(d)

29.(b) 30.(c) 31.(a) 32.(a) 33.(c) 34.(b) 35.(c)

36.(b) 37.(d) 38.(d) 39.(b) 40.(b) 41.(d) 42.(c)

43.(b) 44.(b) 45.(b) 46.(b) 47.(c) 48.(a) 49.(b)

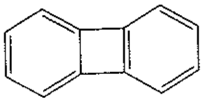
50.(c) 51.(d) 52.(c) 53.(c) 54.(a)

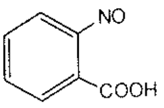
## Mass Spectroscopy
## NET Previous Year's Question

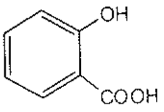
Q1. In the mass spectrum of dodecahedrane $(C_{20}H_{20})$, approximate ratio of the peaks at m / z 260 and 261 is **[NET Dec. 2011]**

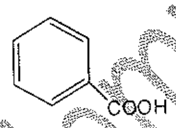
(a) 1 : 1 (b) 5 : 1 (c) 10 : 1 (d) 20 : 1

Q2. Anthranilic acid, on treatment with iso-amyl nitrite furnishes a product which displays a strong peak at $76\,(m/e)$ in its mass spectrum. The structure. The structure of the product is **[NET June 2014]**

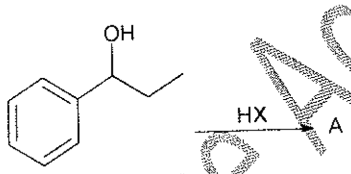
(a) 

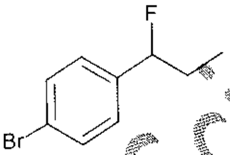
(b) 

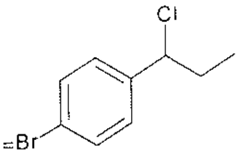
(c) 

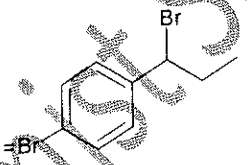
(d) 

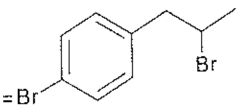
Q3. The mass spectrum of the product A, formed in the following reaction, exhibits $M, M+2, M+4$ peaks in the ratio of about 1 : 2 : 1. The reagent HX and the product A are **[NET June 2014]**



(a) HX = HF and A = 

(a) HX = HCl and A = 

(a) HX = HBr and A = 

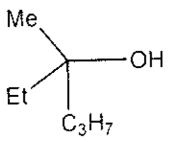
(a) HX = HBr and A = 

Q4. In The mass of metastable ion produced due to decomposition of $F_1^{+}$ in the following mass fragmentation sequence is; **[NET June 2014]**

$$\text{Diethyal-phthalate} \longrightarrow F_1^{+} \longrightarrow F_2^{+} + CO$$

(a) 141.2 (b) 125.4 (c) 45.0 (d) 210.2

Q5. In the mass spectrum of the compound given below, during the $\alpha-$ cleavage, the order of preferential loss of groups is **[NET June 2011]**



(a) $Me > C_3H_7 > Et$ (b) $C_3H_7 > Et > Me$ (c) $Et > Me > C_3H_7$ (d) $Et > C_3H_7 > Me$

Q6. In the mass spectrum of 1,2 – dichloroethane, approximate ratio of peaks at m/z value 98,100,102 will be **[NET Dec. 2015]**

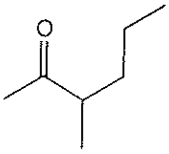
(a) 3 : 1 : 1 (b) 9 : 6 : 1 (c) 1 : 1 : 2 (d) 1 : 2 : 1

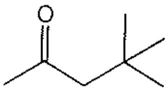
Q7. Mass fragment of $[IrCl]^+$ in mass spectrometry shows three mass peaks at m/z = 226,228 and 230. Given that natural abundances of $^{191}Ir, ^{193}Ir, ^{35}Cl$ and $^{37}Cl$ are 37%, 63%, 76% and 24% respectively, the intensities of the mass peaks in the order **[Net June 2017]**

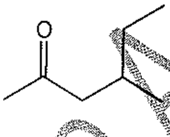
(a) 49.5:100:26.6 (b) 100:49.5:26.6

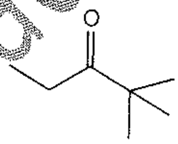
(c) 26.6:100:49.5 (d) 26.6:49.5:100

Q8. Among the following, the compound that gives base peak at $m/z$ 72 in the EI mass spectrum is **[NET Dec. 2017]**

(a)


(b)


(c)


(d)


Q9. Mass spectrum of a compound shows an $[M+2]$ ion peak that is about 4% of $M^+$. This indicates that the compound has one.

(a) Fluorine (b) sulfur (c) bromine (d) chlorine

## Answer Key

1. (b) 2.(b) 3. (c) 4. (b) 5. (b) 6.(b) 7.(a)

8.(a) 9.(b)

## GATE Previous Year's Question

Q1. **Statement:** Bromopyrimidine $(C_4H_3BrN_2)$ exhibits two prominent peaks in the mass spectrum at m/z 158 and 160 in the ratio 1 : 1

**Reason:** There are two basic centres in the molecule, which are protonated.

**Assertion:** There are two isotopes of bromine, $^{79}Br$ and $^{81}Br$, that occur in the ratio of 1 : 1

**[GATE 2004]**

Choose the correct answer from the following four choices.

(a) Both Reason and assertion are correct.

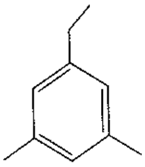
(b)Both Reason and Assertion are wrong

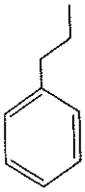
(c) Reason is correct and Assertion is wrong

(d) Reason is wrong but Assertion is correct

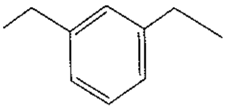
**[GATE 2007]**

Q2. Among the isomers $C_{10}H_{14}$ shown


P


Q


R


S

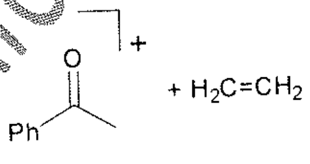
The isomer that can be identified uniquely by mass spectrometry alone is

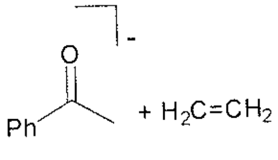
(a) P **(b) Q** (c) R (d) S

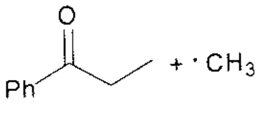
**Linked Answer Type Q3. And Q.4**

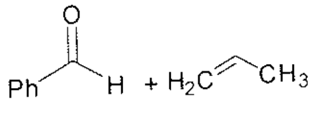
For butyrophenone $(PhCOCH_2CH_2CH_3)$

Q3. The most probable fragmentation observed in the electron impact ionization (EI) mass spectrometry is

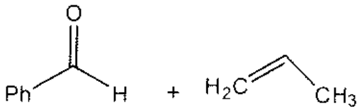
(a)


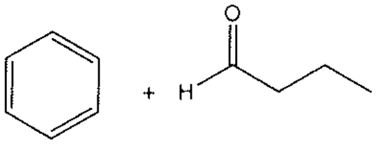
(b)


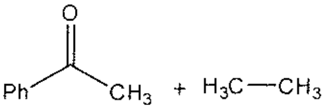
(c)


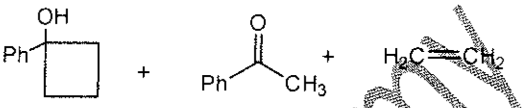
(d)


Q4. Photirradiation leads to the following set of products: **[GATE 2008]**

(a)


(b)


(c)


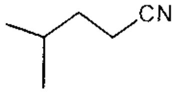
(d)


Q5. The ratio of relative intensities of the two molecular ion peaks of methyl bromide ($CH_3Br$) in the mass spectrum is —————— **[GATE 2012]**

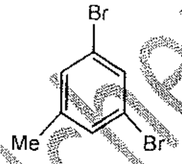
(a) $M^+ : (M+2) = 1.3$ (b) $M^+ : (M+2)^+ = 3:1$

(c) $M^+ : (M+2)^+ = 1:1$ (d) $M^+ : (M+2)^+ = 1:2$

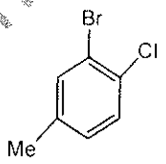
Q6. The $m/z$ value of the detectable fragment formed by Lafferty like rearrangement of the following compound in mass spectrometer is **[GATE : 2014]**



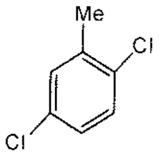
Q7. The mass spectrum of a dihalo compound shows peaks with relative intensities of 1 : 2 : 1 Corresponding to M, M + 2 and M + 4 (M is the mass of the molecular ion), respectively. The compound is **[ GATE 2015]**



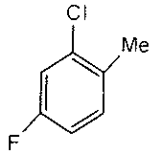
(A)



(B)



(C)



(D)

(a) A (b) B (c) C (d) D

Q8. In the electron ionization (EI) mass spectra, methyl hexanoate, methyl heptanoate and methyl octanoate give. The same base peak. The $m/z$ value of the base peak is **[GATE2018]**

## Answer Key

1. (d) 2.(b) 3. (a) 4. (d) 5. (c) 6.(41) 7.(a)
8.(72)

## TIFR Previous Year's Question

Q1. In the mass spectrum of bromine molecule shows three peaks due to the species $Br_2^+$ with the mass numbers 158,160 and 162. Which isotopes of bromine occur in nuture ? **[TIFR 2010]**

(a) $^{79}$Br and $^{80}$Br (b) $^{80}$Br and $^{81}$Br (c) $^{79}$Br and $^{81}$Br (d) $^{79}$Br,$^{80}$Br and $^{81}$Br

Q2. Electrospray ionization mass spectroscopy produces multiply charged ions of proteins. On application of this technique to hemeprotein it gave a large number of peaks corsponding to different charge-states of the protein. The three consecutive peaks are observed at the $m/z$ values: **[TIFR 2013]**

2016, 1767, 1546

The approximate m/z value of the consecutive fourth speak in the series would be

(a) 1252 (b) 1374 (c) 1498 (d) 1325

Q3. If the peak in the mass spectrum of $C_2F_6$ at mass number 138 is 100 units tall, what will be the heights of the peaks at mass number 139 and 140. **[TIFR 2015]**

( Isotopic abundances: $^{12}C, 98.89\%$ ; $^{13}C, 1.11\%$ ; $^{19}F, 100\%$ )

(a) 2.24 and 0.0126 (b) 1.12 and 0.0126

(c) 50 and 25 (d) 2.24 and 0.025

Q4. Which of the following statements is the best definition of the base peak in a mass spectrum? **[TIFR 2016]**

(a) The molecular ion peak (b) The lowest m/z peak

(c) The highest mass rearrangemention (d) The ion peak greatest intensity

Q5. If the peak in the mass spectrum of $C_2F_6$ at mass number 138 is 100 unit tall, what will be the heights of the peaks at mass number 139and 140. Isotopic abundances: $^{13}C, 98.89\%$ $^{13}C, 1.11\%,$ $^{19}F, 100\%$

**[TIFR 2019]**

(a) 2.24 and 0.0126 (b) 50 and 25 (c) 2.24 and 0.025 (d) 1.12 and 0.0126

Q6. Identify the compound whose molecular ion appears as a pair of equal intensity peaks at m/z = 122 & m/z 124. Large fragment ions are seen at m/z = 43 (base peak) **[TIFR 2019]**

(a) 1 – bromopropane (b) 2 – bromopropane (c) Both A and B (d)) None of these

## Answer Key

1. (c) 2.(b) 3. (a) 4. (d) 5. (*) 6.(*)

## Other Examination Previous Year's Question

Q1. The ratio of M and M + 1 peaks in the mass spectrum of $C_{60}$ is

(a) 1 : 1 (b) 60 : 1 (c) 3 : 2 (d) 1 : 60

Q2. Bromine has two common isotopes, Br - 79 and Br - 81 that occur in an approximate 1 :1 ratio. What would one expect to find in the mass spectrum of bromobenzene?

(a) A large peak at a m/z value of 78.

(b) A large peak at a m/z value of 77 and only one molecular ion peak.

(c) A large peak at m/z value of 77 and two molecular ion peaks of differing heights.

(d) A large peak at a m/z value of 77 and two molecular ion peaks of the same height.

Q3. The base peak in the electron impact mass spectrum (EI MS) of acetophenone is

(a) 120 (b) 105 (c) 77 (d) 65

Q4. In the mass spectrum of bromoform, the ratio of peaks at $m/z$ 250, 252, 254, 256, assuming bromide has isotopes of the masses 79 and 81 in equal abudance, will be

(a) 1 : 1 : 1 :1 (b) 1 : 2 : 2 :1 (c) 1 : 3 : 3 : 1 (d) 1 : 6 : 6 : 1

Q5. 15 In the mass spectrum of dichlorobenzene the ratio of the peaks at m / z 146, 148 and 150, is

(a) 1 : 1 : 1 (b) 3 : 3 :1 (c) 1 : 2 :1 (d) 9 : 6 : 1

Q6. Which one of the following carbonyl compounds will give a fragment ion at m/z = 58 in their mass spectra?

(a) $C_2H_5CH(CH_3)CHO$ (b) $CH_3CH_2CH_2CH_2CHO$

(c) $CH_3CH_2CH_2COCD_3$ (d) $(CH_3)_2CHCH_2CHO$

Q7. Benzene and benzene- $d^6$ (hexadeuterated benzene) may be readily distinguished by:

(a) Thin layer chromatography (b) UV-visible (absorption) spectroscopy

(c) $^{13}C$ NMR spectroscopy (d)Mass spectrometry

Q8. Which technique would you use to quickly distinguish methyl benzoate from phenyl acetate?

(a) $^1H$ NMR (b)Mass spectrometry

(c) Vapor pressure osmometry (d) Elemental analysis.

## Answer Key

1. (c) 2.(d) 3. (b) 4. (c) 5. (d) 6.(a) 7.(d)

8. (b)

## NMR Spectroscopy
## NET Previous Year's Question

Q1. An organic compound $(C_7H_{12}O_2)$ exhibited the following data in the $^1H$ NMR spectrum.

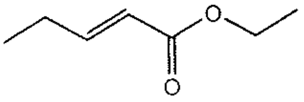
**[NET June 2011]**

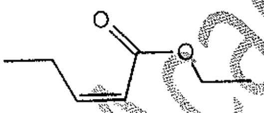
$\delta 7.10(1H, dt, J = 16 \text{ and } 7.2Hz), 5.90(1H, dt, J = 16 \text{ and } 2Hz)$

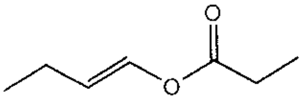
$4.1(2H, q, J = 7.2Hz), 2.10(2H, m), 1.25(3H, t, J = 7.2Hz)$

$0.90(3H, t, J = 7.2Hz)$ ppm

The compound, among the choices given below, is

(a) 

(b) 

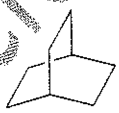
(c) 

(d) 

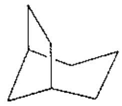
Q2. In the broad decoupled $^{13}C$ NMR spectrum, the number of signals appearing for the bicyclooctane A-C respectively , are

**[NET June 2011]**

(A)



(B)



(C)

(a) Five, four and eight

(b) Three, two and Five

(c) Five, four and five

(d) Three, two and eight

Q3. In the $^{19}F$ NMR spectrum of $PF_5$ the number of singles and multiplicity, at room temperature are

**[NET Dec 2011]**

(a) One, singlet

(b) One, doublet

(c) two, doublet

(d) two singlet

Q4. An organic compound $(MF: C_8H_{10}O)$ exhibited the following $^1H$ NMR spectral data: $\delta 2.5(3H, s), 3.8(3H, s), 6.8(2H, d, J8Hz), 7.2(2H, d, J8Hz)$ ppm. The compound among the choices, is

**[NET Dec. 2011]**

(a) 4 - ethylphenol

(b) 2 - ethylphenol

(c) 4 -methylanisole

(d) 4- methylbenzyl alcohol

Q5. The NMR spectrum of $AX_3$ exhibits lines at $\delta = 2.1$ and 2.3ppm (for A type protons), and $\delta = 4.1, 4.3, 4.5$ and 4.7 ppm (for A type protons), measured from TMS with an instrument operating at 100MHz. The chemical shift (in ppm) of A and X protons and cuping constant (in Hz ) are respectively.

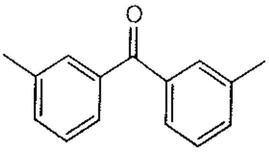
**[NET Dec. 2011]**

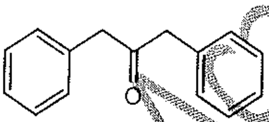
(a) 4.4,2.2 and 20 (b) 2,2,4.4 and 10 (c) 2.2,4.4 and 5 (d) 4.3,2.1 and 20

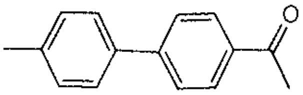
Q6. An organic compound having molecular formula $C_{15}H_{14}O$ exhibited the following $^1H$ and $^{13}C$ NMR spectral data.

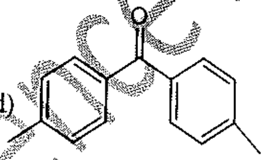
$^1H$ NMR: $\delta 2.4(s), 7.2(d, J = 8Hz), 7.7(d, J = 8Hz)$

$^{13}C$ NMR : $\delta 21.0, 129, 0.130.0, 136.0, 141.0, 190.0$

(a)


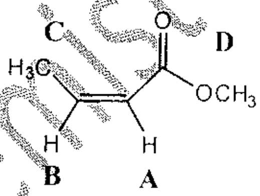
(b)


(c)


(d)


Q7. Appropriate $^1H$ NMR chemical shifts $(\delta)$ for the protons A-D for the following compound are

**[NET Dec. 2011]**



(a) A – 6.8; B – 5.7; C – 3.9;D – 2.1ppm (b) A – 6.8; B – 5.7; C – 2.1; D – 3.9 ppm

(c) A – 5.7; B – 6.8; C – 3.9; D – 2.1 ppm (d) A – 5.7; B – 6.8; C – 1; D – 3.9 ppm

Q8. A compound A having the composition $FeC_9H_8O_3$ shown one signal at 2.5 ppm and another one around 5.0 ppm in its $^1H$ NMR spectrum. The IR spectrum of this compound shows two bands around the 1680 $cm^{-1}$. The compound follows the 18 electron rule of the following statements for A, the correct one is/are

**[NET Dec. 2011]**

(A) It has $\eta^5 - Cp$ group (B) It has terminal CO ligand

(C) It has a $CH_3$ ligand (D) It has Fe - H bond

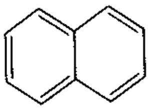
(a) (A) and (B) only (b) (A) and (C) only

(c) (A) and (C) only (d) (B) and (D) only

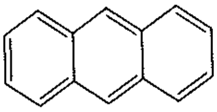
Q9. The uncertainty in the NMR frequency of a compound in liquid state (relaxation time = 1s) 0.1 Hz The uncertainty in the frequency (in Hz) of same compound in solid state (relaxation time = 1s) is **[NET Dec.2011]**

(a) $10^{-4}$ (b) 100 (c) 1000 (d) $10^{-3}$

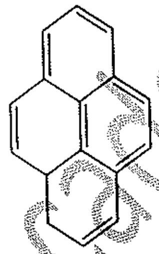
Q10. The number of distinct peak in the proton decoupled $^{13}C$ NMR spectra of the following compounds I - III, respectively, are: **[NET June 2012]**



**(A)**



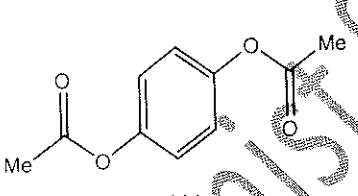
**(B)**



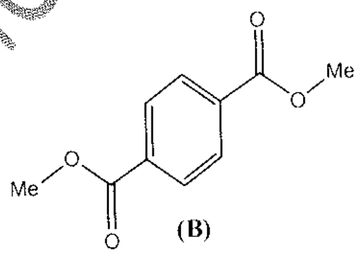
**(C)**

(a) 4,6,8 (b) 3,4,5 (c) 3,5,7 (d) 2,4,6

Q11. Compounds A and B exhibit two singlets, each in their $^1H$ NMR spectra, The expected chemical shifts are at $\delta$ **[NET June 2012]**



**(A)**



**(B)**

(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

**[NET June 2012]**

Q12. Match of the following

| Compound | $^{13}C$ NMR chemical shift ($\delta ppm$) |
|---|---|
| (A) Acetic acid | (i) 95 |
| (B) Acetonitrile | (ii) 115 |
| (C) Acetone | (iii) 175 |
| (D) Carbon tetrachloride | (iv) 205 |

(a) (A) - (iii), (B) - (ii), (C) - (iv), (D) - (i) (b) (A) - (iii), (B) - (iv), (C) - (i), (D) - (ii)

(c) (A) - (i),(B) - (ii), (C) - (iv), (D) - (ii) (d) (A) - (iii), (B) - (i), (C) - (iii),(D) - (iv)

Q13. In the 400 MHz $^1HNMR$ spectrum of organic compound exhibited a doublet. The two lines of the doublet are at $\delta 2.35$ and $2.38\ ppm$ . The coupling constant (J) value is **[NET June 2012]**

(a) 3Hz (b) 6Hz (c) 9Hz (d) 12Hz

Q14. The number of single that appear in the appear in the broadband decoupled $^{13}C$ NMR spectrum of phenanthrene and anthracene, respectively are **[NET June 2012]**

(a) ten and four (b) ten and ten

(c) sevan and four (d) sevan and seven

Q15. The carbonyl resonance in $^{13}C$ NMR spectrum of $[(\eta^5-C_5H_5)Rh(CO)]_3$ ($^{103}$Rh, nucleaspin, I = 1/2, 100%) shows a triplet at $65^\circ C$ owing to the presence of **[NET June 2012]**

(a) Terminal CO (b) $\mu_2-$ CO (c) $\mu_3-$ CO (d) $\eta^5-C_5H_5$

Q16. The metal complex that exhibits a triplet as well doublet in its $^{31}P$ NMR spectrum is **[NET June 2012]**

(a) mer $-[IrCl_3(PPh_3)_3]$ (b) trans $-[IrCl(CO)(PPh_3)_2]$

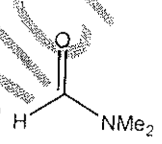
(c) fac-$[IrCl_3(PPh_3)_3]$ (d) $[Ir(PPh_3)_4]$

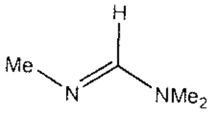
Q17. $^1H$ NMR spectrum of HD would shows **[NET Dec.2012]**

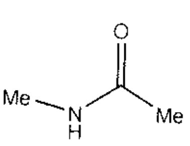
(a) a singlet (b) a doublet

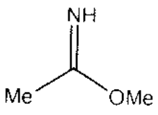
(c) a triplet with intensity ratio 1 : 2 : 1 (d) a triplet with intensity ratio 1 : 1 : 1

Q18. In the $^1H$ NMR spectrum recorded at 293K, an organic compound $(C_3H_7NO)$, exihibited singnals at $\delta 7.8(1H, s), 2.8(3H, s)$ and $2.6(3H, s)$. The compound is **[NET Dec. 2012]**

(a)


(b)


(c)


(d)


Q19. Consider the following statements for [18] annulene

(A) It is aromatic

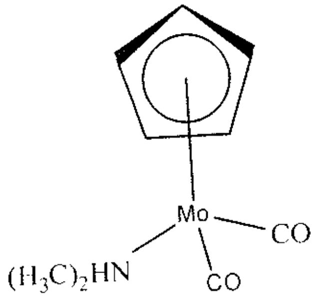
(B) The inner protons resonate at $\delta$ 9.28 in its $^1H$ NMR spectrum

(C) There are six protons in the shielded zone.

(a) A,B,C (b) A and only (c) B and C only (d) A and C only

**[NET Dec. 2012]**

Q20. For the molecule below,



Consider the following statements about its room temperature spectral data.

(A) 1H NMR has singlets at 5.48 and 3.18 ppm

(B) 1H NMR has multiplet at 5.48 and singlet at 3.18 ppm

(C) IR has CO stretching bands at 1950 and 1860 cm$^{-1}$

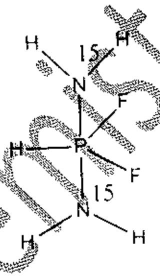
(D) IR has only CO stretching band at 1900 cm$^{-1}$

The correct pair of statements is

(a) A and C (b) B and C (c) A and D (d) B and D

**[NET Dec. 2012]**

Q21. Find out the number lines in the $^{31}$P NMR signal for



(a) 3 (b) 6 (c) 18 (d) 90

**[NET Dec. 2012]**

Q22. 4 - Hydroxybenzoic acid exhibited signals at $\delta 171, 162, 133, 122$ and 116 ppm in its broadband decoupoled $^{13}$C NMR spectrum. The correct assignment of the signals is

(a) $\delta$ 171(C – 4), 162 (COOH), 133( C - 3&5), 122 (C – 1) and 116(C – 2 & 6)

(b) $\delta$ 171 (COOH), 162 (C – 4), 133 ( C – 2 & 6) 122 (C – 1)and 116 (C – 3 & 5)

(c) $\delta$ 171 (C – 4), 162 (COOH), 133 (C – 2 & 6) (C – 1) and 116 (C – 3 & 5)

(d) $\delta$ 171 (COO), 162 (C – 4), 133 (C - 3 & 5), 122 (C – 1) and 116(C – 2 & 6

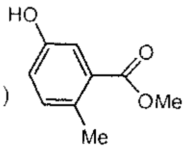
Q23. An organic compound $(C_9H_{10}O_3)$ exhibited the following spectral data **[NET Dec.2012]**

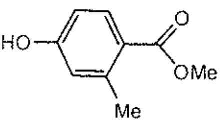
IR : 34000,180cm$^{-1}$

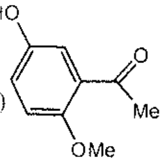
$^1$H NMR : δ7.8(1H, d, J = 8Hz), 7.0(1H, g, J = 8Hz), 6.5(1H, s), 5.8(1H, s, $D_2O$) exchange geable,

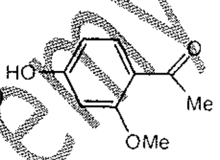
3.9(3H, s), 2.3(3H, s)

The compound is

(a) 

(b) 

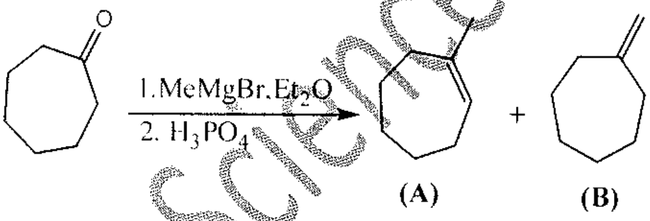
(c) 

(d) 

Q24. An AX system gave 4 lines at 4.72, 4.6, 1.12 and 1.0 ppm away from the TMS using an NMR spectrometer operating at 100MHz. What are the values of $J_{AX}$ ( in Hz ) and $\delta_{AX}$ ( in ppm) respectively **[NET June 2013]**

(a) 12 and 3.6 (b) 6 and 3.6 (c) 12 and 2.86 (d) 6 and 2.86

Q25. Among the following, the correct statements for the following reaction is **[NET June 2013]**



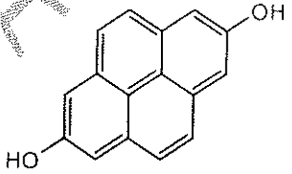
(a) A is major product and it will have five signals the proton decoupled $^{13}$C NMR spectrum

(b) A is the minor product and it will have eight signals in the proton decoupled $^{13}$C NMR spectrum

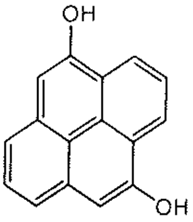
(c)B is the major product and it will have five signals in the proton decoupled $^{13}$C NMR spectrum

(d) B is the minor product and it will have five signals in the proton decopled $^{13}$C NMR spectrum

Q26. In the broad band decoupled $^{13}$C NMR spectrum the number of signals appearing for the two pyrendiols A and B **[NET June 2013]**



**(A)**



**(B)**

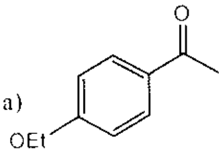
(a) eight and eight (b) eight and sixteen

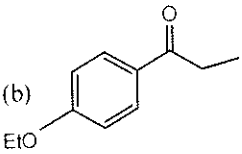
(c) five and ten (d) Five and eight

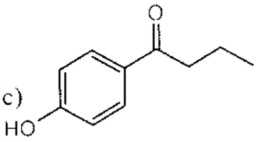
Q27. An organic compound exhibited the following $^{1}H$ NMR spectra data **[NET June 2013]**

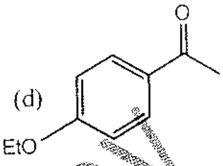
$\delta$ 7.80 (2H,d,J = 8 Hz), 6.80 (2H, d, J = 8Hz), 4.10(2H, q, J = 7.2 Hz) 2.4(3H,s),1.25 (3H, t, J = 7.2Hz)

The compound, among the choice given below is

(a)


(b)


(c)


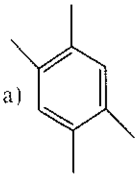
(d)


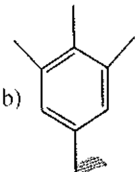
Q28. In NMR spectroscopy the product of the nuclear 'g' factor (g), the nuclear magneton $(\beta_N)$ and the magnetic field strength $(B_0)$ gives the **[NET June 2013]**

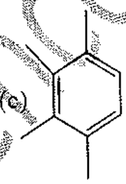
(a) energy of transition from α to β state (b) Chemical shift

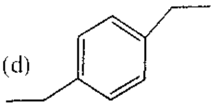
(c) spin-spin coupling constant (d) megnetogyric ratio

Q29. A organic compound having the molecular formula $C_{10}H_{14}$ exhibited two singlets in the $^{1}H$ NMR spectrum. And three signals in the $^{13}C$ NMR spectrum. The compound is **[NET Dec. 2013]**

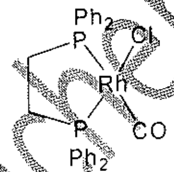
(a)


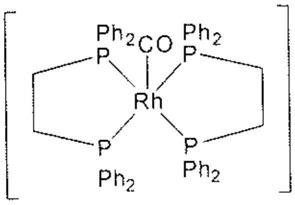
(b)


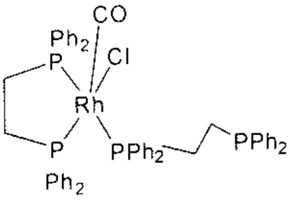
(c)


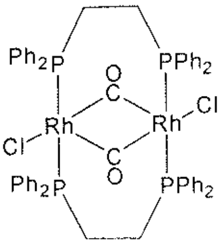
(d)


Q30. Reaction of $Ph_2PCH_2CH_2PPh_2$ with $[RhCl(CO)_2]_2$ in a 2 : 1 molar ratio gives a crystalline solid A. The IR spectrum of complex A shows $\nu_{CO}$ at 1985 $cm^{-1}$. The $^{31}P\{^{1}H\}$NMR spectrum of A consists of two doublets of doublets of equal intensities ($^{103}Rh$ is 100% abundant and $I = 1/2$). The structure of complex A is **[NET Dec. 2013]**

(a)


(b)


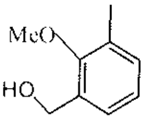
(c)


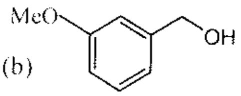
(d)


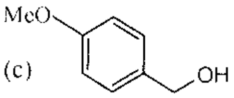
Q31. An organic compound $\left(C_6H_{10}O_2\right)$, which does not change the color of ferric chloride Solution, exhibited the following $^1H$ NMR spectral data: **[NET Dec. 2013]**

$\delta$ 7.3 (1H, t, J = 8Hz), 7.0(1H, d, J = 8 Hz), 6.95(1H,s), 6.9(1H,d,J = 8Hz)

5.3 (1H, brs, $D_2O$ exachangeable), 4.6 (H, s),3.9 (3H,s). Structure of the compound is

(a) 

(b) 

(c) 

(d) 

Q32. Methyl -4 oxopentanoate exchibited signals at $\delta$ 208, 172, 51, 37, 32 and 27 ppm in its $^{13}C$ NMR spectrum. The signalsdue to the methoxy, C1, C4 and C5 carbons are **[NET Dec. 2016]**

(a) OMe – 32; Cl – 208; C4 – 172; C5 - 51

(b) OMe – 51; Cl – 208; C4 – 172; C5 - 32

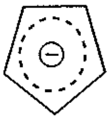
(c) OMe – 32; Cl – 172; C4 – 208; C5 - 51

(d) OMe – 51; Cl – 172, C4 – 208; C5 – 32

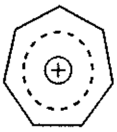
Q33. Given $\gamma\left({}^1H\right) \approx 2.7\times10^8 T^{-1}s^{-1}$ the resonance frequency of a proton in magnetic field of 126 T is close to $\left(\pi = 3.14\right)$ **[NET Dec.2013]**

(a) 60 MHz (b) 110 MHz (c) 540 MHz (d) 780 MHz

Q34. The correct match of the $^1H$ NMR chemical shift $(\delta)$ of the following species compounds is **[NET June 2014]**


(I)


(II)


(III)

(a) I : 5.4; II : 7.2; III : 9.2 (b) I : 9: 2; II : 7.2; III : 5.4

(c) I : 9.2; II : 5.4; III : 7.2 (d) I : 7.2; II : 9.2, II : 5.4

Q35. The $^{19}F$ NMR spectrum of $ClF_3$ shows **[NET June 2014]**

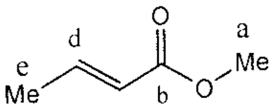
(a) doublet and triplet for a T-shaped structure

(b) singlet s for a trigonal planar structure

(c) singlet for a trigonal pyramidal structure

(d) doublet and singlet for a T-shaped structure

Q36. The correct $^{13}C$ NMR chemical ($\delta$) shift values of carbons labeled a-e in the following ester are **[NET June 2014]**



(a) a : 19; b : 143; C : 167; d : 125; e : 52

(b) a : 52; b : 143; c : 167; d : 125; e : 19

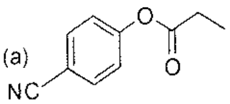
(c) a : 52; b : 167; c : 143; d : 125 : e : 19

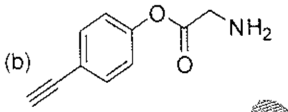
(d) a : 52; b : 167; c : 125; d : 143; e :19

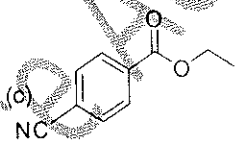
Q37. An organic compound gives following spectral data **[NET June 2014]**

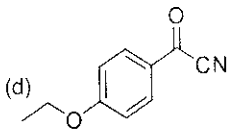
IR: 2210, 1724cm$^{-1}$; $^{1}H$ NMR : 1.4(t, J = 7.1Hz, 3H), 4.4(q, J = 7.1Hz, 2H); $^{13}C$ NMR : $\delta$16, 62, 118, 119, 125, 127, 168

the compound is









Q38. The ratio of the relative intensities of the carbon signals in the first order $^{13}C$NMR spectrum of $CD_3Cl$ is **[NET Dec. 2014]**

(a)1 : 4 : 6 : 4 : 1

(b) 1 : 3 : 3 : 1

(c) 1 :6 : 15 : 20 : 15 : 6 : 1

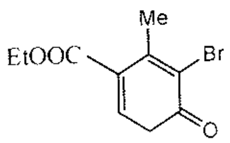
(d) 1 : 3 : 6 : 7 : 6 : 3 : 1

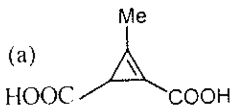
Q39. The following reactions gives a product (recemic) which exhibits the following NMR data **[NET Dec. 2014]**

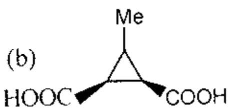
$^{1}H$ NMR:$\delta$2.67(2H,s), 5.60(2H,s)

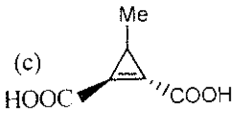
ppm, $^{13}C$ NMR : $\delta$ 170.3, 129.0, 105.0, 25.4 ppm

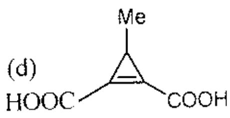
The structure of the product (racemic) is











Q40. An organic compound having molecular formula $C_{10}H_{12}O_2$ exhibits the following spectral data **[NET Dec. 2014]**

IR : $3400(\mathrm{br}), 1600\mathrm{cm}^{-1}$

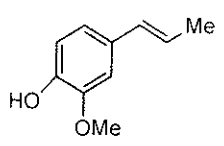
$^1H$ NMR : $\delta 1.85(3H, d, J = 6Hz), 3.8(3H, s), 5.0(1H, s, D_2O$ exchangeable$)$

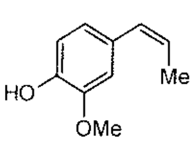
$6.0(1H, dq, J = 18, 6Hz)$

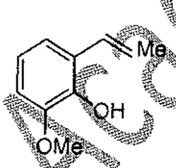
6.28 (1H, d, J = 18 Hz), 6.75 (1H, d, J = 8 Hz), 6.8 (1H, s), 6.90 (1H, d, J = 8 Hz)ppm

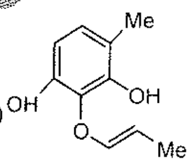
$^{13}C$ NMR : $\delta 146.5, 144.0, 131.0, 130.5, 123.0, 119.0, 114.0, 108.0, 55.0, 18.0$ ppm

The structure of the compound is

(a) 

(b) 

(c) 

(d) 

Q41. A borane (X) is reacted with ammonia to give a salt of borohydride (Y). The $^{11}B$ NMR spectrum of Y consists of a triplet and quintet. The borane X is **[NET Dec. 2014]**

(a) $B_2H_6$ (b) $B_3H_9$ (c) $B_4H_8$ (d) $B_5H_9$

Q42. $^1H$ NMR spectrum of free benzene shows a peak at ~7.2 ppm. The expected chemical shift ( in ppm). The expected chemical shift ( in ppm ) of $C_6H_6$ ligand in $^1H$ NMR spectrum of $[(\eta^6 - C_6H_6)Cr(CO)_3]$ and the reason for it, if an, is/are **[NET Dec. 2014]**

(a) 4.5; disruption of ring current

(b) 9.0 inductive effect

(c) 7.2

(d) 2.5 combination of inductive effect and disruption of ring current

Q43. The nuclear g-factors of $^1H$ and $^{14}N$ are 5.6 and 0.40 respectively. If the magnetic field in an NMR spectrometer is set such that be protons resonates at 700 MHz, the $^{14}N$ nucleus would resonate at **[NET June 2015]**

(a) 1750 MHz (b) 700 MHz (c) 125 MHz (d) 50 MHz

Q44. The $^1H$ NMR spectrum of a dilute solution of a mixture of acetone and dichloromethane in $CDCl_3$ exhibits two singlests of 1 : 1 intensity. Molar ratio of acetone to dichloromethane of thane in the solution is

**[NET June 2015]**

(a) 3 : 1 (b) 1 : 3 (c) 1 : 1 (d) 1 : 2

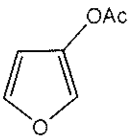
Q45. An organic compounds shows followings spectral data **[NET June 2015]**

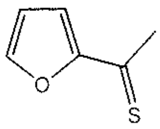
IR $\left(\mathrm{cm}^{-1}\right)$ 1680

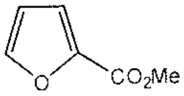
$^{1}\mathrm{H}$ NMR $(\mathrm{CDCl_3})$: $\delta 7.66(\mathrm{m}, 1\mathrm{H}), 7.60(\mathrm{m}, 1\mathrm{H}), 7.10(\mathrm{m}, 1\mathrm{H}), 2.50(\mathrm{s}, 3\mathrm{H})$

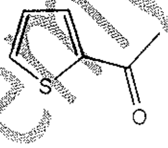
$^{13}\mathrm{C}$ NMR $(\mathrm{CDCl_3})$: $\delta 190, 144, 134, 132, 128, 28\ m/z(\mathrm{EI}): 126(\mathrm{M}^{+}, 100\%), 128(\mathrm{M}^{+}2, 4.9\%)$

The structure of the compound is

(a)


(b)


(c)


(d)


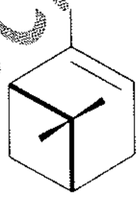
Q46. The $^{119}\mathrm{Sn}$NMR chemical shift (approximately in ppm) corresponding $\left(\eta^{5}-\mathrm{Cp}\right)_2$ Sn (relative to $\mathrm{Me_4Sn}$ ) is **[NET June 2015]**

(a) - 4 (b) +137 (c) + 346 (d) - 2200

Q47. Number of signals in the $^{13}\mathrm{C}\left\{^{1}\mathrm{H}\right\}$NMR spectrum of (R) - 4 - methylpentan-2 - ol are **[NET June 2015]**

(a) 3 (d) 4 (c) 5 (d) 6

Q48. The number of chemical shift non-equivalent protons expected in $^{1}\mathrm{H}$ NMR spectrum of $\alpha$ -pineneis **[NET Dec 2015]**



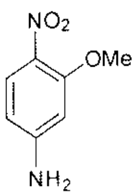
$\alpha$ - pinene

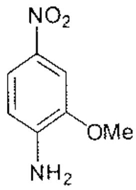
(a) 7 (b) 8 (c) 9 (d) 10

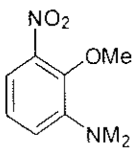
Q49. The structure of the compoundS that matches the $^{1}\mathrm{H}$ NMR data given below is

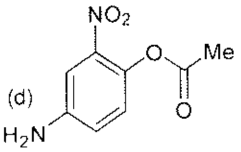
$^{1}\mathrm{H}$ NMR $(\mathrm{DMSO}-d_6)$: $\delta 7.75(\mathrm{dd}, J=8.8, 2.4\,\mathrm{Hz}, 1\mathrm{H}), 7.58(\mathrm{d}, J=2.4\,\mathrm{Hz}, 1\mathrm{H}), 6.70(\mathrm{d}, J=8.8\,\mathrm{Hz}, 1\mathrm{H})$

6.50 (broad s, 2H), 3.80 (s,3H) **[NET Dec 2015]**

(a)


(b)


(c)


(d)


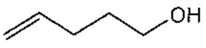
Q50. The $^{1}H$ MNR frequency at 1.0 T is 42.4 MHz. If the gromagnetic ratios of $^{1}H$ and $^{13}C$ are $27 \times 10^{7}$ and $6.75 \times 10^{7} S^{-1}$, respectively, what will be the $^{13}C$ frequency at 1.0 T? **[NET Dec.2015]**

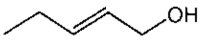
(a) 10.6 MHz (b) 169.9 MHz (c) 42.6MHz (d) 21.3HMz

Q51. In an NMR spectrometer containing a 2.5 T magnet, Larmor, Precession frequency of $^{1}H$ is 100 MHz. The radiofrequency used in this spectrometer has an associated magnetic field strength of $2.5 \times 10^{-4}$ T. The duration of a $90^{0}$ pulse in this instrument is **[NET June 2016]**

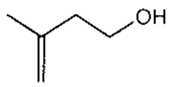
(a) $25 \times 10^{-6}$s (b) $50 \times 10^{-6}$s (c) $25 \times 10^{-5}$s (d) $50 \times 10^{-5}$s

Q52. The correct structure of the compound, which shows following $^{13}C$ NMR DEPT $-135$ data is $^{13}C$ NMR DEPT-135 negative peaks at $\delta$ 30.2, 31.9, 61.8, 114.7 ppm; positive peak at 130.4 ppm **[NET June 2016]**

(a) 

(b) 

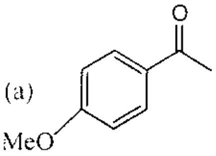
(c) 

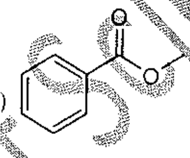
(d) 

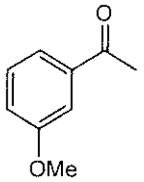
Q53. A compound displays the following spectral data. The correct structure of the compound is IR : 1690 $cm^{-1}$

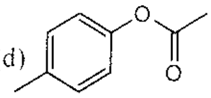
$^{1}H$ NMR : $\delta 2.5(s, 3H), 3.8(s, 3H), 6.9(d, J = 8Hz, 2H), 7.8(d, J = 8Hz, 2H)$ppm

$^{13}C$ NMR$\delta$197,165,130,129,114,56,26ppm **[NET June 2016]**

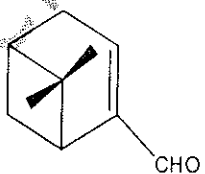
(a) 

(b) 

(c) 

(d) 

Q54. In the $^{1}H$ NMR spectrum of myrtenal, the two methyl groups are expected to display signals at (chemical shift values ($\delta$) in ppm) **[GATE June 2016]**



myrtenal

(a) 1.35 (s, 3H) and 5.0 (s, 3H) (b) 0.74(s, 3H) and 1.33 (s, 3H)

(c) 1.22 (s, 6H) (d) 0.70 (s, 6H)

Q55. The numbers of lines shown by the $BH_3$ part of the molecule $Ph_3P.^{11}BH_3$ in the $^{1}H$ and $^{11}B$ spectra are respectively $[I(^{11}B) = 3/2 : I(^{31}P) = 1/2]$ **[NET June 2016]**

(a) 8 and 8 (b) 4 and 8 (c) 3 and 6 (d) 6 and 3

Q56. In a 200 MHzNMR 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 **[NET Dec. 2016]**

(a) 600 Hz and 30Hz (b) 1200 Hz and 30 Hz

(c) 600 Hz and 10 Hz (d) 1200 Hz and 10 Hz

Q57. $^1H$ NMR spectrum of an organic compound recorded on a 500 MHz spectrometer showed a quartel with line positions at 1759, 1753, 1747, 1741Hz. Chemical shift $(\delta)$ and coupling constant (Hz) of the quartet are **[NET Dec. 2016]**

(a) 3.5 ppm, 6 Hz (b) 3.5 ppm, 12 Hz

(c) 3.6 ppm, 6 Hz (d) 3.6 ppm, 12 Hz

Q58. The expected number of $^{19}F$ NMR spectral lines, including satellites, for $[XeF_5]$ **[NET Dec. 2016]**

$[A\ bundance f\ ^{129}Xe(I = 1/2)\ 26\%]$

(a) two (b) twenty one (c)three (d) one

Q59. $^1H$ NMR spectrum of a mixture of benzene and acetonitrile shows singlets of equal integration. The molar ratio of benzene: acetonitrile is **[NET Dec.2016]**

(a) 1 : 1 (b) 2 : 1 (c) 1 : 2 (d) 6 : 1

Q60. The correct statements in the context of NMR spectroscopy is **[NET Dec. 2016]**

(a) static magnetic field is used to induce transition between the spin states

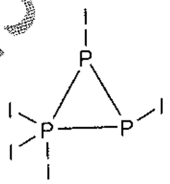
(b) magnetization vector is perpendicular to the applied static magnetic field

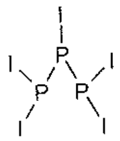
(c) The static magnetic fields is used to create population difference between the spin states

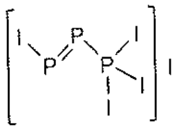
(d) static magnetic field induces spin-spin coupling.

Q61. The reaction between $PI_3$, $PSCl_3$ and zinc powder gives $P_3I_5$ as one the products. The solution state $^{31}P$ NMR spectrum of $P_3I_5$ shows a doublet $(\delta 98)$ and a triplet $(\delta 98)$ . The correct structure of $P_3I_5$ is **[NET Dec. 2016]**

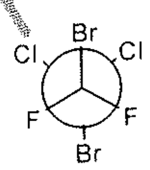
(a) 

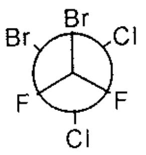
(b) 

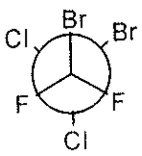
(c) 

(d) 

Q62. Number of lines in the $^{19}F$ NMR spectrum of $F_2C(Br)-C(Br)Cl_2$ at $-120^0C$ assuming it a mixture of static conformations given below, are **[NET Dec. 2016]**





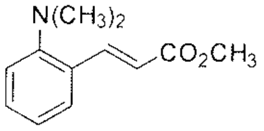


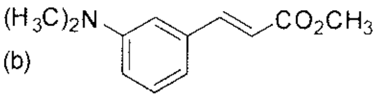
(a) one (b) two (c) four (d) five

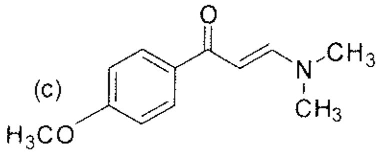
Q63. The compound that exhibits following spectral data is **[NET Dec. 2016]**

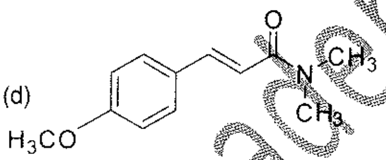
$^1H$ NMR : $\delta$8.0(d, J = 12.3Hz, 1H), 7.7(d, J = 8.0Hz, 2H)

6.8 (d, J = 8.0 Hz, 2 H), 5.8 (d, J = 12.3 Hz, 1H), 3.8(s, 3H), 3.0(s,6H) ppm

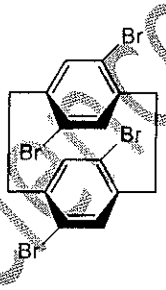
(a)


(b)


(c)


(d)


Q64. Number of signals present in the proton decoupled $^{13}C$ NMR spectrum of the following compound is **[NET Dec.2016]**



(a) four (b) six (c) eight (d) ten

Q65. $^{13}C$ NMR spectrum of DMSO - $d_6$ gives a signal at $\delta$ 39.7 ppm as a **[NET June 2017]**

(a) singlet (b) triplet (c) quintet (d) septet

Q66. The $^{31}P\{^1H\}$NMR spectrum of $2,2,6,6-N_4P_4Cl_4(NMe_2)$ is expected to show **[NET June 2017]**

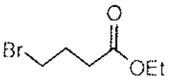
(a) two triplets (b) two doublets

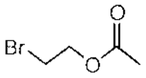
(c) one doublet and one triplet (d) one quartet and one doublet

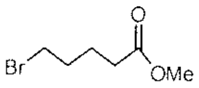
Q67. The correct structure of the compound based on the following characteristic spectral data is **[NET Jun 2017]**
IR: 1736 $cm^{-1}$

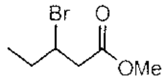
$^1H$ NMR:$\delta$3.59(s,3H), 3.32(t,2H), 2.25(t,2H), 1.85 – 1.45(m,2H), 1.73 – 1.62(m,2H)

$^{13}C$ NMR : $\delta$ 174.0, 51.0, 32.9, 32.9, 32.8, 31.0, 23.0

(a)


(b)


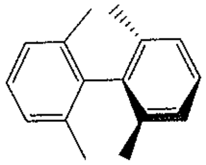
(c)


(d)


Q68. For a certain magnetic field strength, a free proton spin transition occurs at 700MHz. Keeping the magnetic field strength constant the $^{14}N$ nucleus will resonate at $\left(g(p) \approx 5.6g \text{ and } g(^{14}N) \approx 0.4\right)$ **[NET June 2017]**

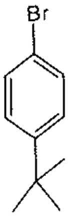
(a) 700 MHz (b) 400 MHz (c) 200 MHz (d) 50MHz

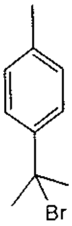
Q69. The number of signals observed in the proton decoupled $^{13}C$ NMR spectrum of the following compound is **[NET Dec. 2017]**



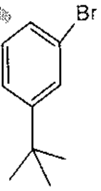
(a) Five (b) Six (c) Ten (d) Thirteen

Q70. The organic compound that displays following data is $^{1}H$ NMR (400MHz) : $\delta$ 7.38(d); 1.29(s) ppm

(a)


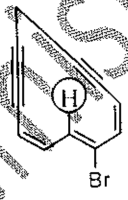
(b)


(c)

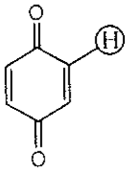

(d)


Q71. The correct match of the circled protons in Column P with $^{1}H$ NMR chemical shift ($\delta$ ppm) in Column Q is **[NET Dec. 2017]**

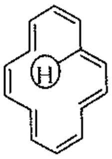
P Q

I


A 6.72

II


B 16.4

III


C -0.61

(a) I – A; II – B; III - C
(b) I – B; I – A; III - C
(c) I – B; II – C; III - A
(d) I – C; II – B ; III - A

Q72. The g- factors of $^{1}H$ and $^{13}C$ are5.6 and 1.4 respectively. For the same value of the magnetic fields strength. If the $^{1}H$ resonates at 600 MHz, the $^{13}C$ would resonate at **[NET Dec. 2017]**

(a) 2400 MHz (b) 600 MHz (c) 150 MHz (d) 38 MHz

Q73. A compound shows following spectral data: **[NET June 2018]**

$^{1}H$ NMR : $\delta 7.9(d, J = 8Hz, 2H), 6.6(d, J = 8Hz, 2H)$,

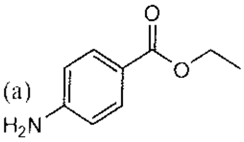
4.3 (q, J = 6.Hz, 2 H) 4.0 (br s, 2H, $D_2O$ exchangeable),

1.4 (t, J = 6 Hz, 3H)

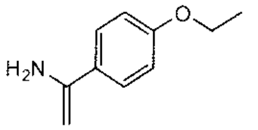
Mass: m / z 165, 137, 120, 92

The correct structure of the compound is

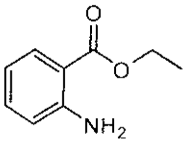
(a)



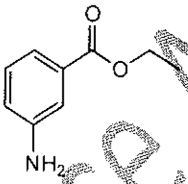
(b)



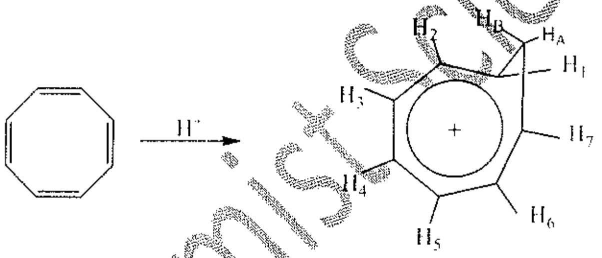
(c)



(d)



Q74. The correct match of protons in Column-A with $^{1}H$ NMR chemical shifts in column-B for the product of the following reaction is **[NET June 2018]**



| Column-A | Column-B ($\delta$ ppm) |
|---|---|
| (P) $H_A$ | (I) 0.3 |
| (Q) $H_B$ | (II) 5.1 |
| (R) $H_{1\&7}$ | (III) 6.4 |
| (S) $H_{2-6}$ | (IV) 8.5 |

(a) P – II, Q – I, R – III, S · IV (b) P – I, Q – II, R – IV, S – III

(c) P – IV, Q – I, R – III, S – III (d) P – II, Q – IV, R – I, S – III

Q75. In the $^{31}P\{^{1}H\}$ NMR spectrum of a diamagnetic complex mer - $[M(PR_3)_3Cl_3]$ ( M = transition metal, I = 0) expected number of resonance(s) is **[NET Dec. 2018]**

(a) Three (b) One (c) Two (d) Six

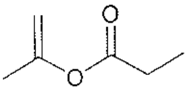
Q76. The $^{31}P\{^{1}H\}$ NMR spectrum of cis - $[Pt(PEt_3)_2Cl_2]$ ( $^{195}$Pt (33.8% abundance) I = ½; its other isotopes are NMR inactive; $^{31}P : I = 1/2$ ) is comprised with satellite peaks of a **[NET Dec. 2018]**

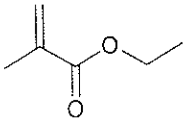
(a) triplet (b) singlet (c) doublet (d) quartlet

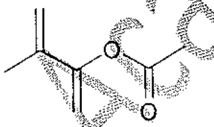
Q77. Structure of the compound displaying following characteristics spectral data. **[NET Dec. 2018]**

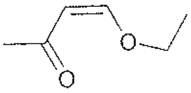
IR : 1720 $cm^{-1}$

$^{1}H$ NMR : 6.2(br, s1H), 5.5(br, s, 1H) 4.2(q, 2H), 2.0(s, 3H), 1.1(t, 3H) is

(a) 

(b) 

(c) 

(d) 

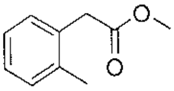
Q78. Partial spectroscopic data is given below for an organic compound **[NET Dec. 2018]**

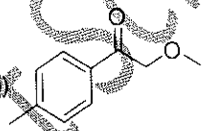
(I) 4 signals between $\delta$ 120 – 150 ppm in $^{13}C$ NMR spectrum

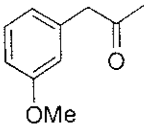
(II) 2 doublets between $\delta$ 6.8-8.5 ppm in $^{1}H$ NMR spectrum

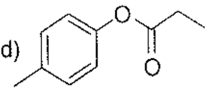
(III) an absorption band at 1724 $cm^{-1}$ in IR spectrum

The structure of the compound is

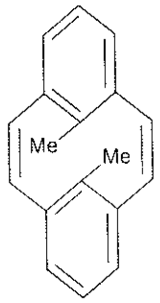
(a) 

(b) 

(c) 

(d) 

Q79. The compound P undergoes a pericyclic reaction under photochemical conditions to give compound Q. In compound Q, The relative stereochemistry and $^{1}H$ NMR chemical shift values of methyl groups (in $\delta$ ppm), respectively, are **[NET Dec. 2018]**



(a) cis; - 5 (b) trans; 17 (c) cis; 17 (d) trans; - 5

## Answer Key

1. (a)
2. (b)
3. (b)
4. (c)
5. (a)
6. (d)
7. (d)
8. (a)
9. (c)
10. (b)
11. (a)
12. (a)
13. (d)
14. (c)
15. (b)
16. (a)
17. (d)
18. (a)
19. (d)
20. (a)
21. (d)
22. (b)
23. (d)
24. (a)
25. (d)
26. (c)
27. (a)
28. (a)
29. (a)
30. (a)
31. (b)
32. (d)
33. (c)
34. (a)
35. (a)
36. (d)
37. (c)
38. (d)
39. (c)
40. (a)
41. (a)
42. (a)
43. (d)
44. (b)
45. (d)
46. (d)
47. (d)
48. (d)
49. (b)
50. (a)
51. (a)
52. (a)
53. (a)
54. (b)
55. (a)
56. (d)
57. (a)
58. (c)
59. (c)
60. (b)
61. (c)
62. (c)
63. (c)
64. (a)
65. (d)
66. (a)
67. (c)
68. (d)
69. (a)
70. (a)
71. (b)
72. (c)
73. (a)
74. (a)
75. (c)
76. (b)
77. (b)
78. (b)
79. (d)

## GATE Previous Year's Question

Q1. The $^{19}F$ NMR spectrum of $PCl_2F_3$ (I for $^{31}P = 1/2$, I for $^{19}F = 1/2$) shows **[GATE 2000]**

(a) Two triplets and two doublets (b) Two triplet and one doublet
(c) Two doublets and one triplet (d) three triplets and one doublet

Q2. The number of signals observed in $^{1}H$ NMR spectrum of 3,5 - dibromotoluene is **[GATE 2001]**

(a) 3 (b) 4 (c) 2 (d) 6

Q3. In comparision to the frequency of the EPR transition, the NMR transition frequency is **[GATE 2001]**

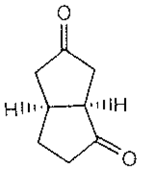
(a) much higher (b) much lower (c) almost same (d) none of these

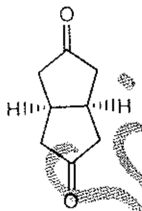
Q4. $^{19}F$ NMR spectrum of meriodional isomer of octahedral $RhCl_3F_3$ complex, $[^{103}Rh(I = 1/2);\ ^{19}F(I = 1/2)]$ assuming $J_{Rh-F} > J_{F-F}$ will show **[GATE 2001]**

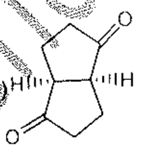
(a) one doublet (b) two doublets and one triplet

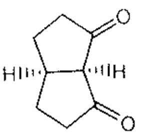
(c) two doublets and two triplets (d) one singlet and two triplets

Q5. Among the bicyclo [3, 3, 0]octanediones given below, which one will exhibit FIVE signals in the broad band decoupled $^{13}C$ NMR spectrum **[GATE 2002]**

(a) 

(b) 

(c) 

(d) 

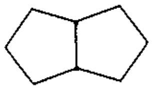
Q6. The sensitivity of a 600 MHz NMR spectrometer is more than that of a 60 MHz spectrometer because **[GATE 2003]**

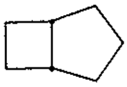
(a) Population of spin states is directly proportional to the applied magnetic field
(b) Population of spin states is inversely proportional to the applied magnetic field.
(c)According to the Bolzamann distribution law, the excess population in the lower spin state increases with increasing applied magnetic field.
(d) The spectral scan width is more for a 600 MHz spectrum compound to a 60 MHz spectrum.

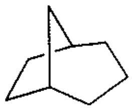
Q7. $^{1}H$ – NMR spectrum of a compound with molecular formula $C_4H_9NO_2$ shows $\delta$ 5.30 (broad, 1H) , 4.10(q, 2H) ,2.80 (d, 3H), 1.20 (t, 20 (t, 3H) ppm. The structures of the compound that is consistent with the above data is: **[GATE 2003]**

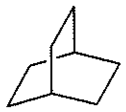
(a) $CH_3NHCOOCH_2CH_3$ (b) $CH_3CH_2NHCOOCH_3$
(c) $CH_3OCH_2CONHCH_3$ (d) $CH_3CH_2OCH_2CONH_2$

Q8. Proton decoupled $^{13}C$ NMR spectrum of a bicyclooctane $(C_8H_{14})$ exhibits only two signals. The structure of the compound is: **[GATE 2004]**

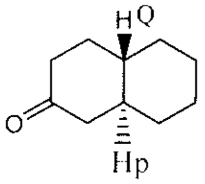
(a) 

(b) 

(c) 

(d) 

Q9. The vicinal coupling constant J expected for the protons $H_p$ and $H_q$ in the compound given below will be in the range **[GATE 2004]**

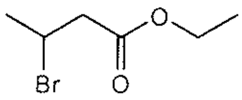


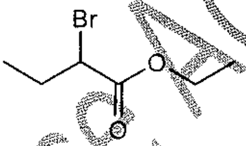
(a) 0 – 2 Hz (b) 4 – 6Hz (c) 8 – 10Hz (d) 12 – 15 Hz

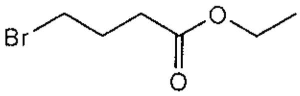
Q10. An organic compound having molecular formula $C_6H_{11}BrO_2$ exhibits the following peaks in $^1H$ NMR spectrum. **[GATE 2004]**

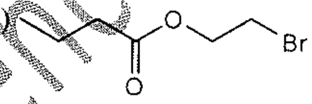
$\delta$ 4.1 (2H, q, J = 7.5 Hz), 4.0 (2H, t, J = 7.5 Hz), 1.5 – 2.2 (4H, m), 1.25 (3H, t, J = 7.5 Hz)

The structure of the compound is:

(a)


(b)


(c)


(d)


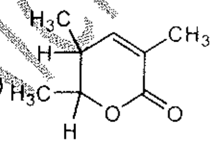
Q11. $^1H$ NMR spectrum of [18] - annulene shows **[GATE 2005]**

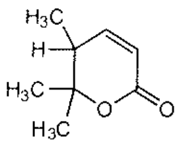
(a) only one peak at $\delta$ 7.2 (18 H) (b) Only one peak at $\delta$ 5.0 (18 H)

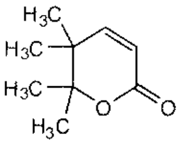
(c) Two peaks at $\delta$ 9.0 (12 H) and $\delta$ - 3.0 (6H) (d) two peaks at $\delta$ 9.0 (6H) and $\delta$ - 3.0 (12 H)

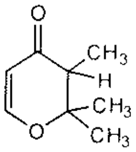
Q12. An organic compound having molecular formula $C_8H_{12}O_2$ exhibits the following peaks in IR and $^1H$ NMR spectra. **[GATE 2005]**

IR: 1720 ($cm^{-1}$) $^1H$ NMR : 6.95(1H, d, J = 8.5Hz)5.90(1H, d, J = 8.5Hz, 4.53(1H,q,J = 6Hz) 1.41(3H, d, J = 6Hz), 1.20 (3H, s), 1.15 (3H, s)

(a)


(b)


(c)


(d)


Q13. Which of the following compounds is expected to show a sharp singlet for one of its protons at $\delta \geq 8$ ppm in $^1H$ NMR spectrum, given that this single remains unaffected on shaking the solution thoroughly with $D_2O$ ? **[GATE 2006]**

(a) $CH_3CO_2H$ (b) $CH_3CONH_6CH_5$

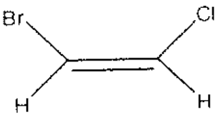
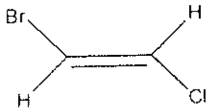
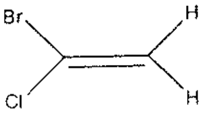
(c) $n-C_6H_{13}C \equiv CH$ (d) $n-C_6H_{13}CHO$

Q14. In the proton decoupled $^{13}C$ and $^{31}P$ NMR spectra of $(CH_3)_3P=O$, the number of lines observed, respectively, are **[GATE 2006]**

(a) two and one (b) one and two

(c) three and one (d) two and two

Q15. Match the structures **List-I** with the coupling constant $\left[{}^1HJ(Hz)\right]$ given in **List –II**

| **List – I** | **List - II** |
|---|---|
| (1)  | (i) ~ 1 Hz |
| (2)  | (ii) ~ 10 Hz |
| (3)  | (iii) ~ 15 Hz |

(a) 1-(i), 2-(ii), 3-(iii) (b) 1-(ii), 2-(iii), 3-(i)

(c) 1-(iii), 2-(ii), 3-(i) (d) 1-(iii), 2-(i), 3-(ii)

Q16. If $ClF_3$ were to be stereochemically rigid, its $^{19}F$ NMR spectrum $\left(I \text{ for } ^{19}F = \frac{1}{2}\right)$ would be (assume that Cl is not NMR active) **[GATE 2008]**

(a) a doublet and a triplet (b) a singlet

(c) a doublet and a singlet (d) two singlets

**Lined Answer Type for Q.17 and Q. 18**

The reaction of $PCl_3$ with methanol in the presence of triethylamine affords compound X. EI mass spectrum of X shows a parent ion peak at m/z = 124. Microanalysis of X shows that it C, H, O and P. The $^1H$ NMR spectrum of X shows a boublet at 4.0 ppm. The separation between the two lines of the doublet is approximately $15\,Hz\left(I \text{ for } ^1H \text{ and } ^{31}P = \frac{1}{2}\right)$

**[GATE 2008]**

Q17. Compound X is

(a) $(CH_3O)_3P$ (b) $(CH_3O)_2P(O)$

(c) $(CH_3O)_2P(O)(OH)$ (d) $(CH_3O)_3PH$

Q18. Upon heating, compound X is converted to Y, which has the same molecular formula as that of X. The $^{1}H$ NMR spectrum of Y shows two doublet centered at 3.0 ppm (separation of two lines ~20Hz) and 4.0 ppm (reparation of two lines ~15 Hz) respectively. **[GATE 2008]**

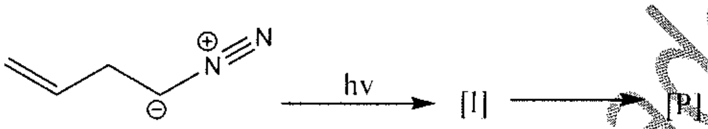
Compound Y is

(a) $(CH_3O)_2P(O)(OH)$ (b) $(CH_3O)_3P(O)$

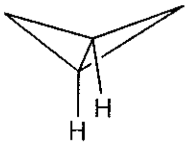
(c) $(CH_3O)_2(CH_3)P(O)$ (d) $(CH_3O)_2(CH_3)P(OH)$

**Linked Answer Q.19 and Q.20** **[GATE 2008]**

In the following reaction,

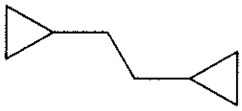


Q19. The reactive intermediate I and the product P are

(a) carbene and


(b) radical and


(c)carbene and


(d) radical and


Q20. The product P shows 'm' and 'n' number of signals in $^{1}H$ and $^{13}C$ NMR spectra, respectively. The value of 'm' and 'n' are

(a) m = 3 and n = 3 (b) m = 2 and n = 3

(c)m = 2 and n = 2 (d) m = 4 and n = 4

Q21. The $^{31}P$ NMR spectrum of $P_4S_3$ Consists of **[GATE 2009]**

(a) a singlet (b) a doublet and triplet

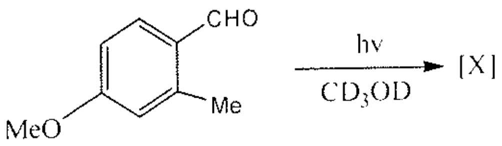
(c) a doublet and quartet (d) two doublets

Q22. The $^{1}H$ NMR spectrum of HD consists of a **[GATE 2009]**

(a) singlet (b) 1 : 1 doublet

(c) 1 : 1 : 1 triplet (d) 1 : 2 : 1 triplet

Q23. In the photochemical reaction **[GATE 2009]**



Formation of the compound X can be inferred by the $^1$H NMR signal at $^1$H NMR spectrum of the strating material:

δ 9.7 (1H, s), 7.8 (1H, d, J = 8.0 Hz), 7.1 – 6.8 (2H, m), 3.9 (3H, s), 2.5 (3H, s) ppm

(a) δ 9.7 ppm (b) δ 7.8 ppm (c) δ 3.9 ppm (d) δ 2.5 ppm

**Common data for Q.24 and Q.25:**

An organic compound $X(C_9H_{10}O)$ exhibited the following spectral data

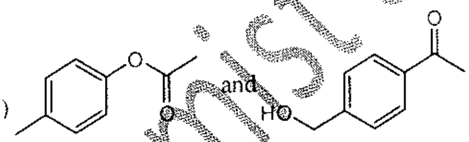
IR: 1680 $cm^{-1}$

$^1$H NMR : δ7.8(2H, d, J7.5Hz), 7.2(2H, d, J = 75 z), 2.7 (3 H, s) and 2.4 (3H, s)

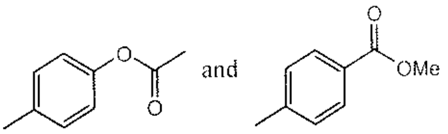
Compound X on treatment with m-choloroperbenzoic acid product two isomeric compound Y (major) and Z (minor)

Q24. Compound Y and Z, respectively, are **[GATE 2009]**

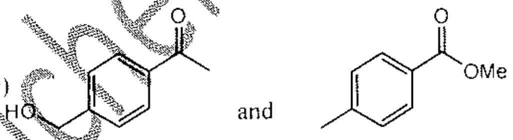
(a)



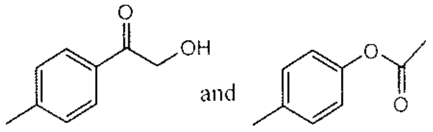
(b)



(c)



(d)



Q25. Compounds Y and Z can be differentiated by carrying out basic hydrolysis, because **[GATE 2009]**

(a) Y produces 4 -methylphenol and Z is unaffected.

(b) Y produces 4 -methylphenol and Z produces 4-methyllbenzoic acid.

(c) Y is unaffected and Z produces 4-methylbenzoic acid.

(d) Y is unaffected and Z produces 4 methylphenol.

**Common data for Q.26 and Q.27:**

Treatment of $W(CO)_6$ with 1 equivalent of $Na(C_5H_5)$ is THF solution gives the ionic compound M Reaction of M with glacial acetic acid results in product N. The $^1H$ NMR spectrum of N displays two singlets of relative intensity 5 : 1 . When N is heated, hydrogen gas is evolved and O is produced; O may also be prepared by refluxing $W(CO)_6$ with cyclopentadiene and $H_2$ is also produced. Treatment of O with an equivalent of $H_2$ produces P. (Use the 18 electron rule as your guide).

Q26. The compound M and N, respectively, are **[GATE 2009]**

(a) $[(C_5H_5)W(CO)_3]Na$ and $[(C_5H_5)W(CO)_3H]$

(b) $[(C_5H_5)W(CO)_4]Na$ and $[(C_5H_5)W(CO)_4H]$

(c) $[(C_5H_5)W(CO)_3]Na$ and $[(C_5H_5)W(CO)_4H]$

(d) $[(C_5H_5)W(CO)_4]Na$ and $[(C_5H_5)W(CO)_3H]$

Q27. The compound O and P, respectively, are **[GATE 2009]**

(a) $[(C_5H_5)W(CO)_3]_2$ and $[(C_5H_5)W(CO)_3Br]$

(b) $[(C_5H_5)W(CO)_3]$ and $[(C_5H_5)W(CO)_2Br(THF)]$

(c) $[(C_5H_5)W(CO)_2(THF)_2]$ and $[(C_5H_5)W(CO)_3Br]$

(d) $[(C_5H_5)W(CO)_3]_2$ and $[(C_5H_5)W(CO)_2Br(THF)]$

**Common data for Q. 28 and Q. 29:**

An organic compound $[X][C_{12}H_6O_3]$ exhibits the following spectral data

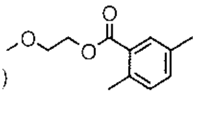
IR:~ 1720 $cm^{-1}$

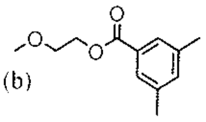
$^1H$ NMR 2.35(s,6H), 3.30(s,3H), 3.83(t,2H), 4.42(t,2H), 7.07(s,1H), 7.58(s,2H)

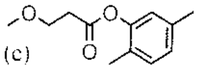
The compound [X] with an excess of MeMgBr gives a 1 : 1 mixture of compounds [Y] and [Z]. The compound [Z] exhibits the following $^1H$ NMR data

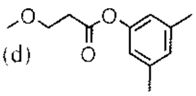
2.0 (bs, 1H) 3.30 (s, 3H), 3.56 (t, 2H), 3.70 (t, 2H)

Q28. The compound [X] is **[GATE 2010]**

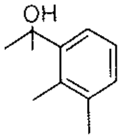
(a)


(b)


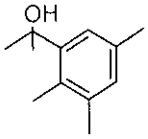
(c)


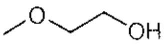
(d)


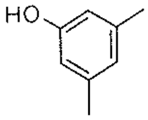
Q29. The compound [Y] is **[GATE 2010]**

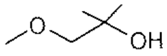
(a) 

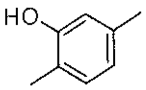
and 

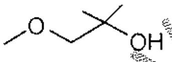
(b) 

and 

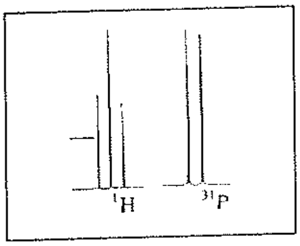
(c) 

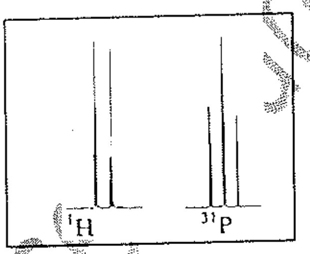
and 

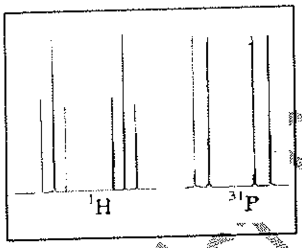
(d) 

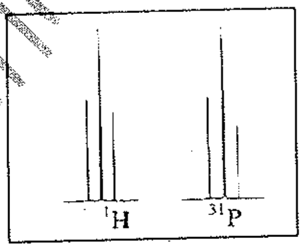
and 

Q30. The correct pair of $^1H$ and $^{31}P$ NMR spectral patterns for $C(H)(F)(PCl_2)_2$ **[GATE 2011]**

(a) 

(b) 

(c) 

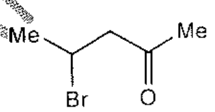
(d) 

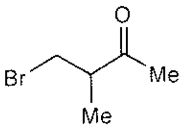
**Statements for linked Answer Q.31 and Q.32**

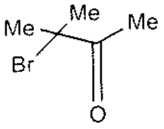
A ketone on treatment with bromine in methanol gives the corresponding monobromo compound [X] having molecular formula $C_5H_9BrO$. The compound [x] when treated with NaOMe in MeOH produces [Y] as the major product. The spectral data for compound [X] are:

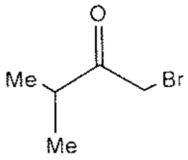
$^1H$ NMR: $\delta$ 1.17 (d, 6H), 3.02 (m, 1H), 4.10 (s, 2H); $^{13}C$ NMR $\delta$ 17, 37, 39, 210.

Q31. The compound [X] **[GATE 2011]**

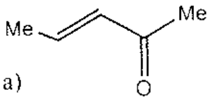
(a) 

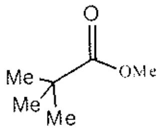
(b) 

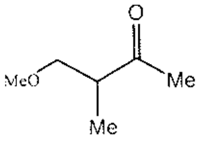
(c) 

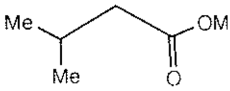
(d) 

Q32. The major product [Y] is **[GATE 2011]**

(a) 

(b) 

(c) 

(d) 

Q33. In the proton decoupled $^{13}C$ NMR spectrum of 7 - norbornanone, the number of signals obtained is **[GATE 2012]**

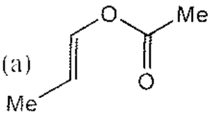
(a) 7 (b) 3 (c) 4 (d) 5

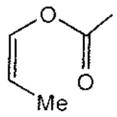
Q34. An organic compound Q exhibited the following spectral data: **[GATE 2013]**

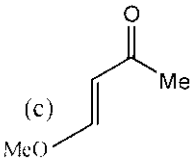
IR: $1760 cm^{-1}$

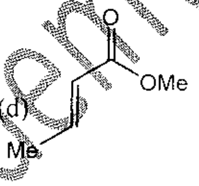
$^1H$ NMR : $\delta$(ppm): 7.2(1H, d, J = 16.0Hz), 5.1(1H, m), 2.1(3H, s), 1.8(3H, d, J = 7.0Hz) 13CNMR : $\delta$(ppm : 170) (carbonyl carbon),

Compound Q is

(a)


(b)


(c)


(d)


**Commond data for Q.35 and Q.36:**

N, N -Demethylformamide (DMF) gives different patterns of signals for the methyl protons whenits $^1H$ NMR spectrum is recorded at different temperatures.

Q35. Match the patterns of the NMR signals given in the Column-I with temperatures guves in the Column-II **[GATE 2013]**

| **Column-I** | **Column-II** |
|---|---|
| (i) Two singlets , for three protons each, at $\delta$ 2.87 and 2.97 ppm | (x) $25^0C$ |
| (ii) One sharp singlet for six protons at $\delta$ 2.92 ppm | (y) $120^0C$ |
| (iii) One broad single for six protons | (z) $150^0C$ |

(a) (i)-(x);(ii)-(y);-(iii)-(z) (b) (i) –(x);(ii)-(z);(iii)-(y)

(c) (i)–(z);(ii);(x); (iii)-(y) (d) (i)-(z);(ii)-(y);(iii)-(x)

Q36. Based on the above data, the calculated difference in the frequencies of the two methyl singlets if the spectrum is recorded on a 300MHz spectrometer, is —————— Hz **[GATE 2013]**

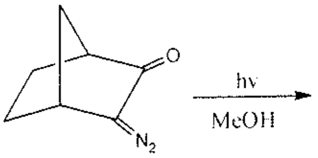
Q37. The number of signals that appear in the proton decoupled $^{13}C$ NMR spectrum of benzonitrile $(C_7H_5N)$ is —————————— **[GATE 2013]**

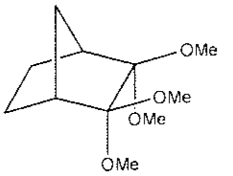
Q38. The set of protons (underline) in $CH_3CH_2CH_2OCH_3$ that would exhibit different splitting patterns in high (500 MHz) and low (60 MHz) fields $^1H$ NMR , is **[GATE 2014]**

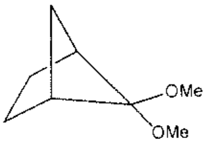
(a) $CH_3CH_2CH_2OCH_3$ (b) $CH_3CH_2CH_2OCH_3$

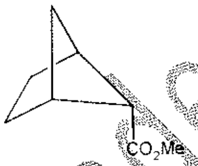
(c) $CH_3CH_2CH_2OCH_3$ (d) $CH_3CH_2CH_2OCH_3$

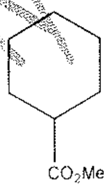
Q39. The product of the following the following reaction gave 6 line $^{13}C$ NMR spectrum with peaks at $\delta$ 175. 52, 50, 46, 37, 33 ppm. The structure of the product is **[GATE 2014]**



(a)


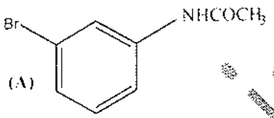
(b)


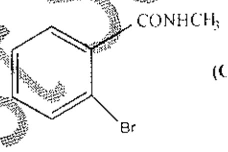
(c)


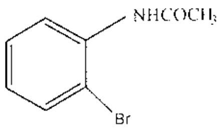
(d)


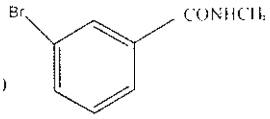
Q40 At room temperature, the number of singlet resonanes observed in the $^1H$ NMR spectrum of $Me_3CO(O)NMe_2$ (NN – dimethyl pivalamide) is ______ **[GATE 2014]**

Q41. The beckmann rearrangement of a bromoatophenone oxime ($C_8H_8BrNO$) gives a major product having the following $^1H$ NMR ($\delta$ ppm): 9.89(s, 1H), 7.88(s, 1H), 7.45(d, 1H, J = 7.2Hz), 7.17 (m, 1H), 7.12 (d, 1H, J = 7.0Hz.), 2.06 (s, 3H). The structure of the product is. **[GATE 2015]**

(A)


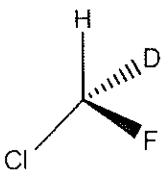
(B)


(C)


(D)


(a) A (b) B (c) C (d) D

Q42. The total number of lines expected (due to spin-spin coupling of proton with fluorine and deuterium nuclei) in the $^1H$ NMR spectrum of the following compound is ______ **[GATE 2016]**

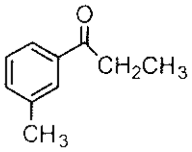


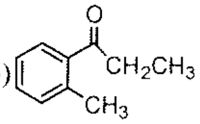
Q43. The larmor frequency of $^1H$ Teals (T) is 42.57 MHz. If the magnetogyric ratio for $^1H$ and $^{13}C$ and are $26.75 \times 10^7$ rad $T^{-1}s^{-1}$ and $6.72 \times 10^7$ rad $T^{-1}s^{-1}$, respectively, the Larmor frequency of $^{13}C$, in MHz, at 1 Tesla will be ______ **[GATE 2016]**

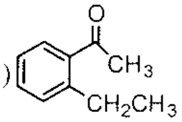
Q44. The structure of the compound having the following characteristics spectral data, is IR: 1690 $cm^{-1}$

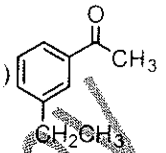
$^1H$ NMR : 1.30(3H, t, J = 7.2Hz); 241(2H, q, J = 7.2Hz); 2.32(3H, s); 7.44(1H, t, -J = 7.0Hz) 7.57 (1H, dt J = 7.0, 3.0 Hz); 7.77 (1H, t, J = 3.0 Hz); 7.90 (1 H, dt, J = 7.0, 3.0 Hz); EI mass m/z 119 (100 %); 57 (80%)

**[GATE 2016]**

(a)


(b)


(c)


(d)


Q45. The $^{19}F$ NMR spectrum of $ClF_3$ when measured $-60^0C$ will be observed as a **[GATE 2016]**

(a) singlet (b) doublet
(c) doublet and triplet (d) doublet of doublet and doublet of triplet

Q46. The $^{13}C$ NMR spectrum of acetone- $d^6$ has a signals at 30 ppm as a septet in the intensity ratio **[GATE 2017]**

(a) 1 : 6 : 15 : 20 : 15 : 6 : 1 (b) 1 : 3 : 6 : 7 : 6 : 3 : 1

(c) 1 : 2 : 3 : 5 : 3 : 2 : 1 (d) 1 : 3 : 7 : 10 : 7 : 3 : 1

Q47. The spectroscopic data for an organic compound with molecular formula $C_{10}H_{12}O_2$ are given below. IR band around 1750 $cm^{-1}$ . **[GATE 2017]**

$^1H$ NMR $\delta$7.3(m:5H), 5.85(q, 1H, J = 7.2Hz), 2.05(s, 3H), 1.5(d, 3H, J = 7.2Hz)ppm . The compound is

(a) methyl2-phenypropinate (b) 1-(phenylethyl) acetate

(c) 2-(phenylethyl) acetate (d) methyl3-phenylpropionate

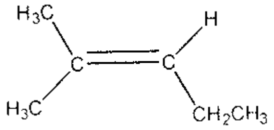
Q48. In the $^1H$ NMR spectrum of an organic compound recorded on a 300 MHz instrument, a proton resonates as a quartet at 4.20 ppm. The individual signals of quartet appear a $\delta$ 4.17, 4.19, 44.21 and 4.23 ppm. The coupling constant J in Hz is ________ **[GATE 2018]**

## Answer Key

1. (a) 2. (a) 3. (b) 4. (*) 5. (d) 6. (c) 7. (a)
8. (d) 9. (c) 10. (c) 11. (c) 12. (c) 13. (d) 14. (a)
15. (c) 16. (a) 17. (a) 18. (c) 19. (a) 20. (c) 21. (c)
22. (c) 23. (a) 24. (b) 25. (b) 26. (a) 27. (a) 28. (b)
29. (b) 30. (c) 31. (d) 32. (c) 33. (b) 34. (a) 35. (b)
36. (30) 37. (5) 38. (b) 39. (c) 40. (3 to 3) 41. (a)
42. (5.99 to 6.01) 43. (10.67 to 10.71) 44. (a) 45. (c) 46. (b)
47. (b) 48. (6)

## TIFR Pervious Year's Question

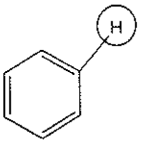
Q1. How many absorption lines will the following naturally occurring compound have in its proton-decupled $^{13}C$ NMR spectrum **[TIFR 2010]**



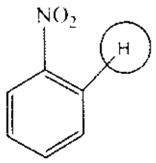
(a) 3 (b) 4 (c) 5 (d) 6

Q2. For each of compounds below, choose the one in which the indicated hydrogen is farthest upfield in a proton NMR spectrum: **[TIFR 2010]**

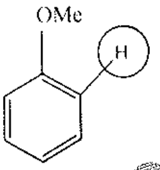
(A)



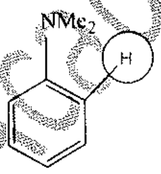
1



2

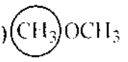


3

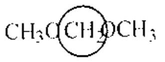


4

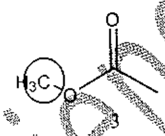
(B)

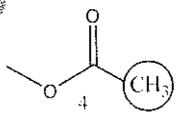


1

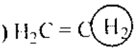


2



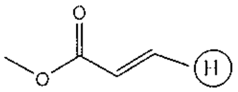


(C)



1

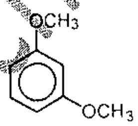
2



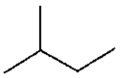
3

(a) A3 or A4,Cl (b) Al, B2, C3 (c) A2, B3, C2 (d) A4, Bl, Cl

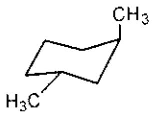
Q3. At room temperature, which of the molecules are expected to give five NMR lines in the proton-decoupled $^{13}C$ NMR spectrum **[TIFR 2010]**



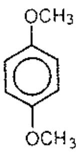
(i)



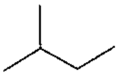
(ii)



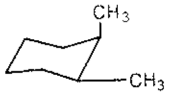
(iii)



(iv)



(v)



(vi)

(a) Only 1 and 3 (b) only 2 and 6 (c) only 3 and 6 (d) All of the above

Q4. The $^{13}C$ NMR spectrum of a compound shows 6 peaks and the $^{1}H$ NMR spectrum shows 5 peaks. Which of the following is this compound **[TIFR 2011]**

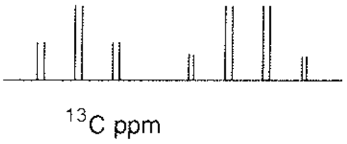
(a) $CH_3-CH(CH_3)-CH(CH_3)-CH(CH_3)-CH_3$

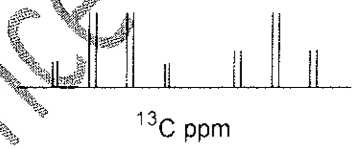
(b) $CH_3-C(CH_3)_2-CH_2-CH_2-CH_3$

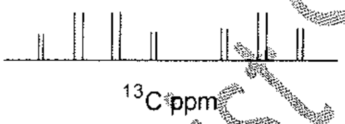
(c) $CH_3-CH(CH_3)-CH_2-CH_2-C(CH_2)_2-CH_3$

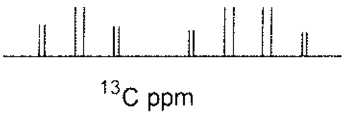
(d) $CH_3-CH(CH_3)-CH_2-CH_2-CH_3$

Q5. Which of the following most closely resembles the $^{13}C$ NMR spectrum of ethanol Assume a scalar coupling of 150 Hz among the $^{1}H$ and the $^{13}C$ nuclei within a functional group, a scalar coupling of 50 Hz between the $^{13}C$ nuclei , a static magnetic field of 11.7 T and a temperature of 300K. **[TIFR 2012]**

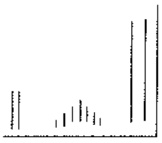
(a) 

(b) 

(c) 

(d) 

Q6. Which of the following compounds would give the $^{1}H$ NMR spectrum shown below **[TIFR 2012]**



(a) $CH_3CH(CH_3)CH_2X$

(b) $CH_3C(CH_3)_2CH_2CH_2X$

(c) $CH_3CH_2(CH_3)CH_2X$

(d) $CH_3CH_2CH(CH_3)X$

Q7. The proton NMR spectrum of saturated hydrocarbon shows a single absorption line at 1.42 ppm with respect to TMS at room temperature. The area of the line is equivalent to 12 protons. Solely based o this observation, what are the tentative inferences you can draw about the nature of the hydrocarbon?

**[TIFR 2012]**

(a) It is a pure compound i.e., there are no impurities present.

(b) More than one conformation of the molecules may be present and they are undergoing rapid interconversion.

(c) The hydrocarbon is cyclohexane.

(d) All of the above

Q8. The $^1H$ NMR spectrum of a compound with molecular formula $C_3H_7NO$ shows the following features: **[TIFR 2013]**

| | | | |
|---|---|---|---|
| Chemical shift (ppm) | 6.50 | 2.25 | 1.10 |
| Sphape | Broad singlet | quartet | triplet |

Which of the following is in agreement with this information?

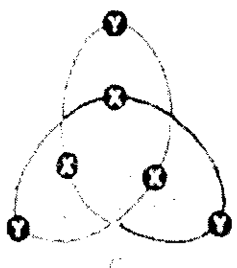
(a) $(CH_3)_2C=NOH$ (b) $CH_3COCH_2NH_2$

(c) $CH_3CH_2CONH_2$ (d) $HCO(NOH_2)_2$

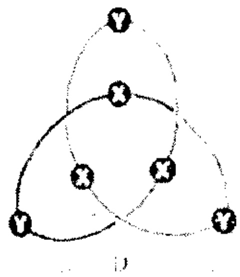
Q9. The two fine-structure components of a nuclear magnetic resonance transition are observed at chemical shifts of 2.142 and 2.208ppm in a 300 MHz spectrometer Calculate the coupling constant **[TIFR 2014]**

(a) 19.8 Hz (b) 0.0666Hz (c) 6.6 Hz (d) data is insufficient

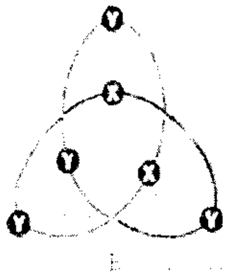
Q10. Molecular knots have been observed in DNA and Proteins. Although synthetically challenging, a few purely organic molecular knots have also been reported in the literature. One such elusive knot is the trefoil knot. An organic trefoil knot was prepared by reacting two structurally distinct components X and Y. The reaction mixture contained four product as shown in the figure below **[TIFR 2015]**



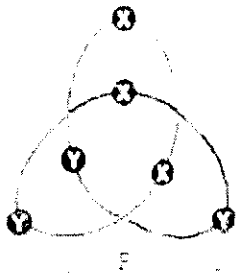
C



D



E



F

Which spectra will afford distinguishable spectral features for (1) C and D? And (2) E and F

(a) Circular Dischroism Spectra for C and D; $^1H-NMR$ for E and F

(b) $^1H-NMR$ and $^{13}C-NMR$ spectra for C and D; Circular Dichroism for E and F

(c)Absorbance and Emission Spectra for C and D; Circular Dichroims for E and F

(d) Infra Red spectra for C and D; Circular Dichroism for E and F +

Q11. Neopentyl chloride, $(CH_3)_3CCH_2Cl$ reacts with a strong base (sodium amide) to produce a new compound. This compound has two $^1H$ NMR singlets at $\delta 0.20$ppm and $\delta 1.05$ppm (intensity ratio = 2 : 3. What is the Most probable structure of this compound? **[TIFR 2016]**

(a) 2 -methyl - 2 - butene (b) 1,1 – dimethylcyclopropane

(c) methylcyclobutane (d) cyclopentane

Q12. The $^1H$ NMR of 1,1 dibromoethane consists of two well-separated signals, one large and another one small. Which one of the following statements is correct? **[TIFR 2016]**

(a) The large signal is a quartet and the small single is doublet

(b) The large signal is a triplet and the small signal is a singlet

(c)The large signal is a singlet and the small singal is a trplet

(d) the large signal is a doublet and the small signal is a quartet.

Q13. A $C_5H_{12}O_2$ compound has strong infared absorption at 3300 to 3400 cm$^{-1}$. The $^1H$ NMR spectrum has three singlets $\delta 0.9, \delta 3.45$ and $\delta 3.2$ 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 $\delta$ 100 ppm. Which of the following compounds best fits this data **[TIFR 2016]**

(a) 1,5 -pentanediol (b) 1,3 -dimethoxypropane

(c) 2,2 – dimethyl-1,3 -propanediol (d) 2,4 -pentanediol

Q14. The $^1H$ NMR spectrum of a compound A shows doublet and a septet. Which one of the following statements is TRUE? **[TIFR 2016]**

(a) The spectrum is consistent with A containing a $CH_3CH_2CH_2$ group

(b) The spectrum is consistent with A being $(CH_3)_2CHCl$

(c) The spectrum is consistent with A Containing a $CH_3CH_2$ group

(d) The spectrum is consistent with A being $(CH_2)_3CCl_2$

Q15. A compound of formula $C_5H_{12}$ gives one signal in the $^1H$ NMR and two singnals in the $^{13}C$ NMR spectra. The compound is **[TIFR 2016]**

(a) pentane (b) 2-methylbutane

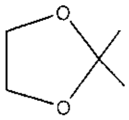
(c) 2,2 – dimethylpropane (d) cannot tell without more information

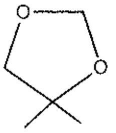
Q16. Predict the multiplicities for hygrogens on Cl, C3 and C4 of butanone associated with the spin-spin coupling in its $^1$H NMR spectrum **[TIFR 2017]**

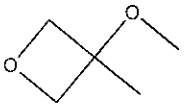
(a) H's on Cl: Singlet; H's on C3: Doublet H's on C4: Triplet
(b) H's on Cl: Singlet; H's on C3: Triplet; H's on C4 : Quartet
(c) H's on Cl: singlett; H's on C3 Quartet; H's on C4 Triplet
(d) H's on Cl Triplet; H's on C3: Doublets H's on C4, Triplet

Q17. An organic compound has the following spectroscopic properties: Mass spectrometry: m/z (very small), 87 and 43 are the largest ions; $^1$H NMR $\delta$1.4 and 3.9 ppm (both singlets, intensity ratio 3 :2 $^{13}$C NMR: $\delta$108.64 and 25 ppm Infrared spectroscopy; several strong absorptions in the 1000 to 1300 cm$^{-1}$ region

Which of the following the most likely formula of this compound? **[TIFR 2017]**

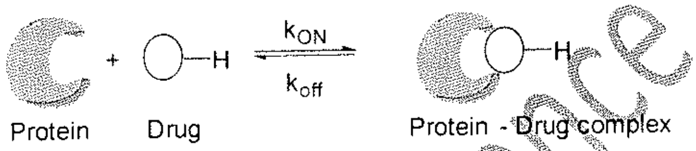
(a) 

(b) 

(c) 

(d) 

Q18.



**[TIFR 2017]**

NMR spectroscopy can be used to assay for drug binding to certain protein targets. One of the primary objectives of any binding assay is the quantifaction of the free and the bound form of a drug molecule at a certain concentration of the protein target. Let us assume that the fully bound drug exhibits $^1$H chemical shift of $\delta_A$ while that of the free formm resonates at $\delta_B$ 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 linewidth of the observed transition (s) will be different from the free form of the drug.

(b) There will be two resonances obtained in the NMR spectrum Protein-Drug complex: one of the free form while other for the bound frorm.

(c) We will see a single resonance at a position $\delta_{eff}$ which is in between $\delta_A$ and $\delta_B$.

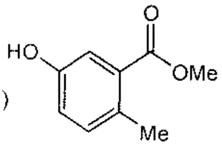
(d) Varying the concentration of the drug molecule while observing the NMR signatures will provide an estimate of the binding constant.

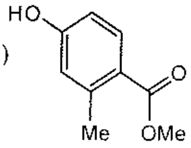
Q19. A compound with molecular formula $C_5H_{12}O_2$, has strong infrared absorption at $3300$ to $3400$ $cm^{-1}$. The $^1$H NMR spectrum showed three singlets at $\delta 0.90, \delta 3.45$ and $\delta 3.20$ $ppm$ with relative areas $3:2:1$. Addition of $D_2O$ to the sample eliminates the lower field signal. The $^{13}$C NMR spectrum shows three singnals all higher than 100 ppm. Which of the following compounds best fits this data? **[TIFR 2017]**

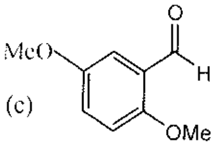
(a) 1,5-pentanediol (b) 1,3-demethoxypropane

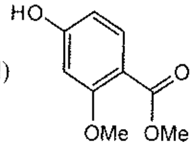
(c) 2,2 -demethyl-1,3-propandiol (d) 2,4 – pentanediol

Q20. An organic compound $(C_9H_{10}O_3)$ exhibited the following spectral data: IR : 3400.1680cm$^{-1}$ $^1$H-NMR:$\delta$7.8 (1 H, doublrd, J = 8Hz), 6.5 (1 H singlet) , 5.8 (1 H, signment, $D_2O$ exchangeable) 3.9 (3 H, singlet), 2.3 (3H, singlet). The compound is, **[TIFR 2018]**

(a)


(b)


(c)


(d)


Q21. A bottle contains hydrogen molecule in gaseous state. The nuclear wavefunctoin of this hydrogen gas is given by **[TIFR 2018**

$$\frac{1}{\sqrt{2}}\left(\alpha(1)\beta(2)-\beta(1)\alpha(2)\right)$$

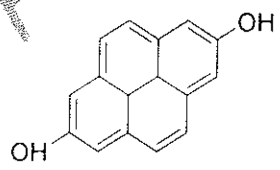
What would be the NMR spectrum of this hydrogen gas, assuming that the wavefunction does not change during recording of the NMR spectrum?

(a) A single NMR peak
(b) Two NMR peaks, each is a doublet
(c) Three NMR peaks, with relative intensities 1 : 2 : 1
(d) No NMR lines

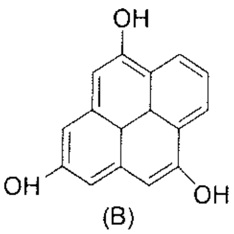
Q22. Identify the organic molecule which contains 66.6% carbon, 11.1% hydrogen. In infra-red spectrum of the molecule, bands are observed at 2941-2857, 1715 and 1640 cm$^{-1}$. In proton NMR, three signals appeared at (i) 7,52 (q, 2H) , (ii) 7.88 (s, 3H), (iii) 8.93 (t, 3H) in ppm scale. **[TIFR 2019]**

(a) Ethyl ketone (b) 2-Butanol
(c) 1-Butanladehyde (d) None of them

Q23. In the broadband decoupled $^{13}$C NMR spectrum, the number of signals appearing for the two pyrenediols A and B **[TIFR 2019]**



(A)



(B)

(a) five and eight (b) eight and eight (c) eight and sixteen (d) five and ten

## Answer Key

1. (c)
2. (c)
3. (b)
4. (c)
5. (a)
6. (a)
7. (d)
8. (c)
9. (a)
10. (a)
11. (b)
12. (d)
13. (c)
14. (b)
15. (c)
16. (c)
17. (a)
18. (b)
19. (c)
20. (d)
21. (d)
22. (*)
23. (d)

## Other examination previous Year's Question

Q1. The chemical shifts of a doublet signal for a proton in a spectrum are 4.08 and 4.06 using a 400 MHz NMR spectrometer. The coupling constant (in Hz) is.

(a) 0.02 (b) 8.0 (c) 8.14 (d) 10.0

Q2. The $^1H$ NMR spectrum of 1,4-dimethoxybenzene will have

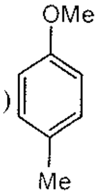
(a) ten singlets (b) two singlets

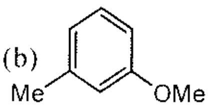
(c) two doublets and one singlets (d) two doublets and two singlets

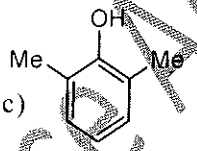
Q3. The pattern of $^1H$ NMR spectrum of 14 - dichlorobenzene is:

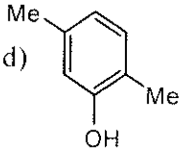
(a) AX (b) AM (c) AB (d) $A_2$

Q4. An organic compound with molecular formula $C_8H_{10}O$ exhibited 6 peaks in its broad-band decoupled $^{13}C$ NMR spectrum. The possible structure of the compound is:

(a)


(b)


(c)


(d)


Q5. The $^1H$ NMR spectrum of molecular has three distinct resonance at approximately, 3.4 ppm (a triplet with an intensity of 2 units), 1.6 ppm (a multiplet with intensity of 2 units). And at 1.0 ppm ( a triplet with an units). The molecule could be

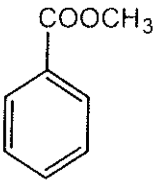
(a) $(CH_3CH_2CH_2)_2O$ (b) $CH_3CH_2Cl$

(c) $CH_3CH_2CH_2CH_3$ (d) $CH_3PCl_2$

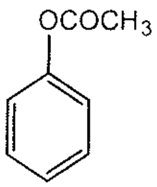
Q6. The number of singles expected for the compounds m-and p-dichlorobenzenes in the broadband decoupled $^{13}C$ NMR spectra are, respectively,

(a) 6 and 4 (b) 4 and 4 (c) 4 and 2 (d) 3 and 2

Q7. In the $^1H$ NMR spectra, signals due to methy groups in isomeric compounds I and II appear respectively at $\delta$.



I



II

(a) 1.25 and 3.9 (b) 3.9 and 2.1 (c) 3.9 and 7.25 (d) 7.25 and 2.1

Q8. The low temperature $^{19}$F NMR spectrum of $IF_5$ molecule in solution should exhibit which of the following patterns? (Ignore any magnetic coupling effects to the iodine nucleus).

(a) One singlet (b) One doublet and one quintet

(c)One singlet and one quintet (d) One quartet and one triplet

Q9. How many signals will be observed in the proton decoupled $^{13}$C NMR for hexamethylbenzene?

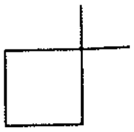
(a) 1 (b) 2 (c) 3 (d) 4

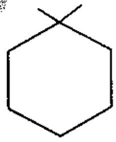
Q10. The $^1$H NMR spectrum of an organic compound of molecular formula $C_4H_8$ exhibited only a singlet at $\delta = 1.9$ ppm. The compound is:

(a) 1 - butane (b) cis-2-butene

(c) trans- 2- butene (d) cyclobutane

Q11. The strength of the coupling between germinal protons in the following molecules



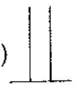
(a) Increases as the size of the ring increases

(b) Decreases as the size of the ring increases

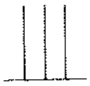
(c)Remains the same

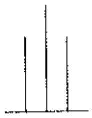
(d) No relation between the size of the ring and the coupling

Q12. The expected spectral pattern in the proton coupled $^{13}$C NMR spectrum of a mixture of equal weights of $CHCl_3$ and $^{13}CHCl_3$ would be

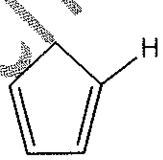
(a) 

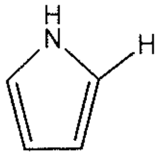
(b) 

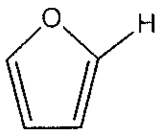
(c) 

(d) 

Q13. The increasing order of chemical shift of the indicated proton in the following series of compounds is







(a) I < II < III (b) III < II < I (c) I < III < II (d) II < III < I

Q14. The $^1H$ NMR spectrum of $(\eta^5 - C_5H_5)$ Fe recorded at room temperature has

(a) One singlet (b) One multiplet (c) Two singlets (d) Two multiplets

Q15. An organic compound with molecular formula $C_3H_6Cl_2$ exhibits only one singal in the $^1H$ NMR spectrum. The compound is:

(a) 2,2 -dichloropropane (b) 1,2 - dichloropropane

(c) 1,3 -dichloropropane (d) 1,1 - dichloropropane

Q16. The $^1H$ NMR chemical shift of $CH_3F, CH_3Cl, CH_3Br$ and $CH_3I$ are

(a) 2.16,2.68,3.05,4.26 (b) 4.26,3.05,2.16,2.68

(c) 4.26,3.05,2.68,2.16 (d) 2.16,3.05,2.68,4.26

Q17. The fine structure and intensity ratios expected in the proton NMR spectrum of $^{14}NH_4^+$ ion (for $^{14}N, I = 1$) are

(a) singlet (b) boublet, 1 : 1

(c) triplet, 1 :1 : 1 (d) triplet 1 : 2 : 1

Q18. In the $^1H$ NMR spectrum of toluene, the resonance due to $CH_3$ group is expected at

(a) $\delta$ 0.5 (b) $\delta$ 1.25 (c) $\delta$ 2.5 (d) $\delta$ 3.5

Q19. For any NMR active nucleus, the magnitude of radiofrequency required for observing nuclear magnetic resonance phenomenon depends on

(a) Strength of the magnetic fields.

(b) Choice of the nucleus

(c) Both on magnetic fields strength and choice of the nucleus.

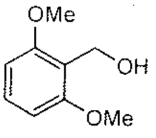
(d) The nuclear energy levels.

20. In the proton NMR spectrum, an organic compound exhibited the following spectral data

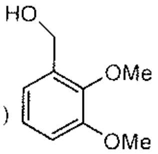
$\delta$ 7.2 (1H, dd, J = 8 and 1.5 Hz), 6.8 (1H, d, J = 1.5 Hz), 6.7 (1H, d, J = 8 Hz), 4.9 (2H, s), 3.9 (3H, s), 3.85 (3H,s), 3.5 (1H, br s, exchangeable with $D_2O$)

The compound among the choice given below is

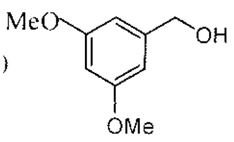
(a)



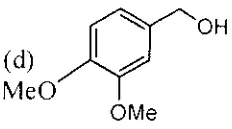
(b)



(c)



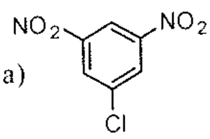
(d)

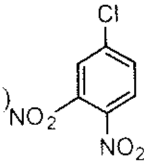


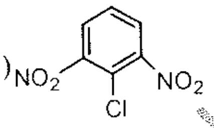
Q21. In the broadband decoupled $^{13}$Carbon NMR spectrum, the number of singals expected for bicycle $[2.2.1]-$ heptanes is

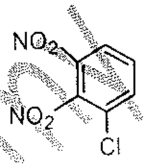
(a) 2 (b) 3 (c) 5 (d) 7

Q22. Which of the following dinitrochlorobenzens exhibits two singlets its $^{1}$H NMR spectrum?

(a) 

(b) 

(c) 

(d) 

Q23. In the broad band decoupled $^{13}$C NMR spectrum, the number of signals appear for (a) catechol, (b) resorcinol and (c) hydroquinone, respectively are

(a) six, four and two (b) six, six and four

(c) three, four and four (d) three, four and two

Q24. The $^{31}$P NMR spectrum of $PF_4N(CH_3)_2$ at room temperature and low temperature (173 K) respectively shows (assume that N and H do not couple)

(a) triplet and quintet (b) quintet and triplet

(c) quintet and triplet of triplets (d) triplet and triplet of triplets

Q25. The order of chemical shift ( $\delta$ value) in the $^{1}H$ NMR spectrum of crotonaldehyde is

(a) Olefinic > CHO > Me (b) CHO > Me > Olefinic

(c) CHO > Olefinic > Me (d) Olefinic > Me > CHO

Q26. How many signals would you expect to see for 1,4 - dinitrobenzene in its $^{1}$H NMR spectra?

(a) One in its $^{1}$H NMR and two in its $^{13}$C NMR spectra.

(b) Two in its $^{1}$H NMR and three in its $^{13}$C NMR spectra

(c)Two in its $^{1}$H NMR and one its $^{13}$C NMR spectra

(d) One in its $^{1}$H NMR and one in its $^{13}$C NMR spectra.

Q27. Which of the following will occur farthest downfields?

(a) The hydrogens of benzens (b) The hydrogens of dimethyl ether

(c) The hydrogens of ethene (d) The hydrogens of ethyne

Q28. How can $CH_3CH_2-C(=O)-OCH_3$ and $CH_3-C(=O)-OCH_2CH_3$ be distinguished by $^1H$ NMR ?

(a) The signals for each compound will have different multiplicities.

(b) Only $CH_3-C(=O)-OCH_2CH_3$ will have a singlet, a triplet, and a quarted.

(c) Only $CH_3CH_2-C(=O)-OCH_3$ will have a singlet, a triplet, and a quartet.

(d) It is by the multiplicity of the signals appearing farthest, downfield

Q29. How many singnals will vinyl chloride have in its $^1H$ NMR spectrum?

(a) 1 (b) 2 (c) 3 (d) 4

Q30. Which of the following compounds shows(s) three signals its $^1H$ NMR spectrum?

(a) 2 - chloro -2- methylbutane (b) 3 - chloropentane

(c) 2 - cholopentane (d) (a) and (b)

Q31. How many signals does 2,2,4 - trimethylpentane have in its $^1H$ NMR spectrum?

(a) 2 (b) 3 (c) 4 (d) 5

Q32. Why does the signal for the hydrogen bonded to oxygen in ethanol appears as a triplet in pure ethanol and as a signlet in ethanol that contains a trace amount of acid.?

(a) Spin exchange cause spin decoupling (b) Electron exchange cause spin coupling

(c)Photon exchange causespin decoupling (d) Chemical exchange cause spin decouling

Q33. In the $^1H$ NMR spectrum of $CH_3CH_2Cl$, the quartet for the $CH_2$ group has a coupling constant of 7 Hz What is the coupling constant for the $CH_3$ triplet?

(a) 0 (b) 3.5 (c) 7 (d) 10.5

Q34. Which of the following is not a true statement ?

(a) 'Clean " splitting patterns require the chemical shift difference between peaks to be at least 10 times the coupling constant.

(b) Coupling constants do not depend on the operating frequency of the NMR.

(c)There are more hert/ ppm on a 360 - MHz NMR than on a 60 - MHzNMR

(d) Spectra taken at higher operating frequency have higher resolution.

Q35. $^{1}H$ NMR spectra of $(CH_3)_2O.CH_3F$ and RCOOH show chemical shift $(\delta)$ in ppm at

(a) 3.27, 4.30 and 10.8 respectively (b) 4.30, 3.27 and 10.8, respectively

(c)3.27, 10.8 and 4.30 respectively (d) 10.8, 4.30 and 3.27, respectively

Q36. How many different types of protons (given unique chemical shift in $^{1}H$ MNR are present in styrene?

(a) 3 (b) 4 (c) 5 (d) 6

Q37. The low temperature $^{1}H$ NMR spectrum of the the Fischer carbene complex $\left[(CO)_5Cr(C(COH_3)Me)\right]$ shows for the methoxy group

(a) Two singlet of inequal intensity

(b) Four resonances in the ratio $1:3:3:1$ due to coupling with Me group

(c) One single resonance for the methyl group

(d) Three peaks due to different environments for each H on the $CH_3$ group

Q38. The multiplicity of the signal in the $^{31}P-NMR$ spectrum of $PD_3$ is:

(a) Singlet (b) Quartet with equal intensity

(c) Septet with unequal intensities (d) Septet with equal intensities

Q39. In the broad decoupled $^{13}C$ NMR spectrum the number of single appear for (a) catechol, (b) resorcinol and (c) hydroquinone, respectively are

(a) six, four and two (b) six, six and four

(c) three, four and four (d) three, four and two

Q40. Which techinique can be used to readily distinguish between isophthalic and terephthalic acids?

(a) $^{13}C$ NMR spectroscopy (b) IR spectrosocopy

(c) Mass spectroscopy (d) UV-Vis spectroscopy

Q41. Cis and trans cinnamic, acids can be most readily distinguished and identified by,

(a) IR spectra (b) UV- spectra

(c) Chemical shift of the olefinic hydrogens

(d) Coupling constant of the olefinic hydrogens.

## Answer Key

1. (b) 2. (b) 3. (d) 4. (a) 5. (a) 6. (c) 7. (b)

8. (b) 9. (b) 10. (d) 11. (a) 12. (a) 13. (a) 14. (a)

15. (a) 16. (c) 17. (c) 18. (b) 19. (c) 20. (d) 21. (b)

22. (a) 23. (d) 24. (c) 25. (c) 26. (a) 27. (a) 28. (d)

29. (c) 30. (d) 31. (b) 32. (c) 33. (c) 34. (c) 35. (a)

36.(d) 37. (b) 38. (c) 39. (d) 40.(a) 41. (d)

## Molecular Spectroscopy

## NET/JRF Year's Question

Q1. In IR spectrum of $\left[Co(CN)_5H\right]^{3-}$ the Co-H stretch is observed at $1840\,cm^{-1}$. The Co-D stretch in $\left[Co(CN)_5D\right]^{3-}$ will appear at nearly **[NET June 2011]**

(a) $1300\ cm^{-1}$ (b) $1400\ cm^{-1}$ (c) $1500\ cm^{-}$ (d) $1600\ cm^{-1}$

Q2. The rotational constant of $^{14}N_2$ is $2\ cm^{-1}$. The wave number of incident radiation in a Raman spectrometer is $20487\ cm^{-1}$. What is the wave number of first scattered stoke line $\left(in\ cm^{-1}\right)$ of $^{14}N_2$? **[NET June 2011]**

(a) 20479 (b) 20475 (c) 20499 (d) 20495

Q3. The $Q$ band in the vibrational spectrum of acetylene is observed in the **[NET June 2011]**

(a) C-C stretching mode (b) C-H symmetric stretching mode

(c) Bending mode (d) C-H antisymmetric stretching mode.

Q4. The vibrational energy levels, $\upsilon''=0$ and $\upsilon'=1$ of a diatomic molecule are separated by $2143\ cm^{-1}$. Its anharmonicity $\left(\omega_e x_e\right)$ is $14\ cm^{-1}$. The values of $\omega_e\left(in\ cm^{-1}\right)$ and first overtone $\left(cm^{-1}\right)$ of this molecule are respectively **[NET Dec. 2011]**

(a) 2143 and 4286 (b) 2157 and 4286 (c) 2157 and 4314 (d) 2171 and 4258

Q5. The molecule that will show Raman spectrum, but not IR spectrum, among the following is **[NET Dec. 2017]**

(a) $H_2$ (b) HCl (c) BrCl (d) $CS_2$

Q6. For a diatomic molecule $AB$, the energy for the rotational transition form $J=0$ to $J=1$ state is $3.9\ cm^{-1}$. The energy for the rotational transition form $J=3$ to $J=4$ state would be **[NET June 2012]**

(a) $3.9\ cm^{-1}$ (b) $7.8\ cm^{-1}$ (c) $11.7\ cm^{-1}$ (d) $15.6\ cm^{-1}$

Q7. For the vibrational Raman spectrum of a homonuclear diatomic molecule, the selection rule under harmonic approximation is **[NET June 2012]**

(a) $\Delta v = 0$ only (b) $\Delta v = \pm 1$ only (c) $\Delta v = \pm 2$ only (d) $\Delta v = 0, \pm 1$

Q8. In the vibrational spectrum of $CO_2$ the number of fundamental vibrational modes common in both infrared and Raman are **[NET Dec. 2012]**

(a) Three (b) Two (c) One (d) Zero

Q9. The relative population in two states with energies $E_1$ and $E_2$ satisfying Boltzmann distributuion is given by $n_1/n_2=(3/2)\exp\left[-(E_1-E_2)/k_BT\right]$. The relative degeneracy $g_2/g_1$ is **[NET Dec. 2012]**

(a) $2$ (b) $2/3$ (c) $3/2$ (d) $3$

Q10. The absorption spectrum of $O_2$ shows a vibrational structure that becomes continuum at $56875\ \text{cm}^{-1}$. At the continuum, it dissociates into one ground state atom $(O_g)$ and one excited state atom $(O_e)$. The energy difference between $O_e$ and $O_g$ is $15125\ \text{cm}^{-1}$. The dissociation energy $(\text{in cm}^{-1})$ of ground state of $O_2$ is: **[NET Dec. 2012]**

(a) $\dfrac{56875}{15125}$ (b) $\dfrac{15125}{56875}$ (c) $72000$ (d) $41750$

Q11. The vibrational frequency and anharmonicity constant of an alkali halide are $300\ \text{cm}^{-1}$ and $0.0025$ respectively. The position $(\text{in cm}^{-1})$ of its fundamental mode and first overtone are respectively. **[NET Dec. 2012]**

(a) $300, 600$ (b) $298.5, 595.5$ (c) 301.5, 604.5 (d) $290, 580$

Q12. In the presence of an external magnetic field (normal Zeeman effect) the transition ${}^1D_2 \rightarrow {}^1P_1$ splits into **[NET Dec. 2012]**

(a) $9$lines (b) $8$ lines (c) $7$lines (d) $6$ lines

Q13. The equilibrium population ratio $(n_j/n_i)$ of a doubly-degenerate energy level $(E_j)$ lying $2$ unit higher than a lower non-degenerate energy level $(E_i)$ assuming $K_BT=1$ unit, will be **[NET June 2013]**

(a) $2e^{-2}$ (b) $2e^{2}$ (c) $e^{2}$ (d) $e^{-2}$

Q14. The atomic masses of fluorine and hydrogen are $19.0$ and $1.0$amu, respectively ( 1amu $=1.67\times10^{-27}$ kg ). The bond length of $HF$ is $2.0\,\overset{0}{A}$. The moment of inertia of $HF$ is **[NET Dec. 2013]**

(a) $3.2\times10^{-47}\ \text{kg m}^2$ (b) $6.4\times10^{-47}\ \text{kg m}^2$

(c) $9.6\times10^{-47}\ \text{kg m}^2$ (d) $4.8\times10^{-47}\ \text{kg m}^2$

Q15. The $C=O$ bond length is $120$ pm in $CO_2$. The moment of the inertia of $CO_2$ would be close to (masses of C and O are $1.9\times10^{-27}$kg and $2.5\times10^{-27}$kg, respectively) **[NET June 2014]**

(a) $1.8\times10^{-45}\,kgm^2$ (b) $3.6\times10^{-45}\,kgm^2$ (c) $5.4\times10^{-45}\,kgm^2$ (d) $7.2\times10^{-45}\,kgm^2$

Q16. Bond lengths of homonuclear diatomic molecules can be determined with the help of both **[NET Dec. 2014]**

(a) Rotational and vibrational spectroscopy

(b) Rotational and rotional Raman spectroscopy

(c) Rotational Raman and electronic spectroscopy

(d) Vibrational and electronic spectroscopy

Q17. If the component of the orbital angular momentum along the molecular axis of a heteronuclear diatomic molecule is non-zero, the rotational-vibrational spectrum will show **[NET Dec. 2017]**

(a) P and R branches only (b) P and Q branches only

(c) Q and R branches only (d) All the P,Q and R branches.

Q18. If the bond length of a heteronuclear diatomic molecule is greater in the upper vibrational state, the gap between the successive absorption lines of P - branch **[NET Dec. 2014]**

(a) Increase non-linearly (b) Decreases non-linearly

(c) Increase Linearly (d) Decrease linearly

Q19. Intense band generally observed for a carbonyl group in the IR spectrum is due to **[NET June 2015]**

(a) The force constant of CO bond is large

(b) The force constant of CO bond is small

(C) There is no change in dipole moment for CO bond stretching

(d) The dipole moment change due to CObond stretching

Q20. The symmetry rotor among the following is **[NET June 2015]**

(a) $CH_4$ (b) $CH_3Cl$ (c) $CH_2Cl_2$ (d) $CCl_4$

Q21. The spectroscopic technique, by which the ground state dissociation energies of diatomic molecules can be estimated, is **[NET June 2015]**

(a) microwave spectroscopy (b) infrared spectroscopy

(c) UV-visible absorption spectroscopy (d) X-ray spectroscopy

Q22. The molecule with the smallest rotational constant (in the microwave spectrum) among the following is **[NET Dec. 2015]**

(a) $N \equiv CH$ (b) $HC \equiv CCl$ (c) $CCl \equiv CF$ (d) $B \equiv CCl$

Q23. The spectroscopic technique that can distinguish unambiguously between trans-1, 2-dichloroethylene and cis-1, 2-dichloroethylene without any numerical calculate is **[NET Dec. 2015]**

(a) microwave spectroscopy (b) UV- visible spectroscopy

(c) X-ray photoelectron spectroscopy (d) $\gamma$- ray spectroscopy

Q24. If the reduced mass of a diatomic molecule is doubled without changing its force constant, the vibrational frequency of the molecule will be **[NET Dec. 2015]**

(a) $\sqrt{2}$ times the original frequency (b) $\frac{1}{\sqrt{2}}$ times the vibrational frequency

(c) twice the original frequency (d) unchanged

Q25. Upon application of the weak magnetic field, a line in the microwave absorption spectrum of rigid rotor splits into 3 lines. The quantum number (J) of the rotational energy level form which the transition originates is **[NET June 2016]**

(a) 0 b) 1 (c) 2 (d) 3

Q26. The rotational constant and the fundamental vibrational frequency of $HBr$ are respectively, $10 cm^{-1}$ and $2000 cm^{-1}$. The corresponding values for $DBr$ approximately are **[NET Dec. 2016]**

(a) $20\ cm^{-1}$ and $2000\ cm^{-1}$ (b) $10\ cm^{-1}$ and $1410\ cm^{-1}$

(c) $5\ cm^{-1}$ and $2000\ cm^{-1}$ (d) $5\ cm^{-1}$ and $1410\ cm^{-1}$

Q27. Among the following, both microwave and rotational Raman active molecule is **[NET Dec. 2016]**

(a) $CH_4$ (b) $N_2O$ (c) $C_2H_4$ (d) $CO_2$

Q28. Vibrations of diatomic molecules are usually modelled by a harmonic potential. If the potential is given by $x^2$ the correct statements is **[NET Dec. 2016]**

(a) force is 2x and force constant 2 (b) force is – 2x and force constant is 2

(c) force is 2x and forces constant is – 1 (d) force is – 2x and force constant is – 1

Q29. The $v = 0$ to $1$ vibration-rotation spectrum of a diatomic molecule exhibits transition for $R(0), R(1), P(1)$ and $P(2)$ lines at $2241, 2254, 2216$ and $2203\ \text{cm}^{-1}$, respectively. Form this data, we conclude that the molecule **[NET June 2017]**

(a) has rigid rotation and harmonic vibration (b) has anharmonic vibration

(c) has rotational-vibrational interaction (d) is effected by nuclear spin-stastics

Q30. The first electronic absorption band maximum of a polar and relatively rigid aromatic molecule appears at $310\text{nm}$ but its flurescence maximum in acetonitrile solution appears with a large Stokes shift at $450\ \text{nm}$. The most likely reason for the Stokes shift is **[NET June 2017]**

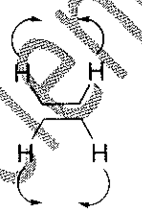
(a) large change in molecular geometry in the excited state

(b) increase is dipole moment of the molecule in the excited state

(c) decrease in polarizability of the molecule in the excited state

(d) lowered interaction of the excited molecule with polar solvent

Q31. The normal mode ethylene represented, by the figure below, is **[NET Dec. 2017]**



(a) only IR active (b) only Raman active

(c) both IR and Raman active (d) neither IR nor Raman active

Q32. The pair contains a spherical top and a symmetric top, among the following, is **[NET Dec. 2017]**

(a) $CH_4, CH_2Cl_2$ (b) $Ch_2Cl_2, CH_3Cl$ (c) $CH_3Cl, CH_4$ (d) $CH_4, C(CH_3)_4$

Q33. Assuming harmonic approximation, the energy change for the reaction $HCl + D_2 \rightarrow DCl + HD$ in $\text{cm}^{-1}$ is (the vibrational frequency data in $\text{cm}^{-1}$ is given in the table below) **[NET June 2018]**

| HCl | $D_2$ | DCl | HD |
|---|---|---|---|
| 2885 | 2990 | 1990 | 3627 |

(a) $-258$ (b) $+258$ (c) $-129$ (d) $+129$

Q34. The transition moment integral for rotational transition between $J=1;M_J=0$ and $J=2;M=0$ states for a diatomic molecule along the z-axis is proportional to **[NET June 2018]**

(a) $\int_0^{\pi}\cos^2\theta\left(3\cos^2\theta\text{-}1\right)d\theta$ (b) $\int_0^{\pi}\cos^2\theta\left(3\cos^2\theta\text{-}1\right)\sin\theta d\theta$

(c) $\int_0^{\pi}\cos\theta\left(3\cos^2\theta\text{-}1\right)\sin\theta d\theta$ (d) $\int_0^{\pi}\cos\theta\left(3\cos^2\theta\text{-}1\right)\sin^2 d\theta$

Q35. A symmetric top molecule, among the following, is **[NET June 2018]**
(a) ethylene (b) allene (c) butatriene (d) hexatriene

Q36. In the pure Raman rotational spectrum of $^{16}O_2$, whose electronic ground state is $^3\sum_g$ transition to/from **[NET June 2018]**
(a) even $J$ levels are missing (b) odd $J$ levels are missing
(c) all $J$ levels appear (d) none of the $J$ levels appear

Q37. In third and fourth lines in the rotational Raman spectrum of CO are separated by 8 $cm^{-1}$. The CO bond length is given by **[NET Dec. 2018]**

(a) $\sqrt{\frac{h}{16\pi^2\mu c}}$ (b) $\sqrt{\frac{3h}{32\pi^2\mu c}}$ (c) $\sqrt{\frac{h}{32\pi^2\mu c}}$ (d) $\sqrt{\frac{5h}{32\pi^2\mu c}}$

Q38. A molecule $AB_2$ shows the following IR and IR Raman spectra

| $\bar{v}\left(cm^{-1}\right)$ | IR | Raman |
|---|---|---|
| 2215 | Vs, PR | S, depol. |
| 1250 | Vs, PR | Vs, pol |
| 560 | S, PQR | - |

The structure of the molecule is **[NET Dec. 2018]**

(a) Linear symmetruical $\left(D_{\infty h}\right)$ (b) Bent symmetrical $\left(C_{2v}\right)$

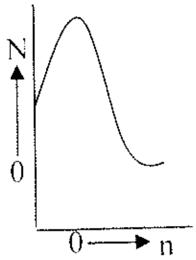
(c) Linear asymmetrical $\left(2_{\infty v}\right)$ (d) Bent asymmetrical $\left(C_s\right)$

## Answer Key

| | | | | | | |
|---|---|---|---|---|---|---|
| 1. (a) | 2. (b) | 3. (c) | 4. (d) | 5. (a) | 6. (d) | 7. (b) |
| 8. (d) | 9. (b) | 10. (d) | 11. (b) | 12. (a) | 13. (a) | 14. (b) |
| 15. (d) | 16. (c) | 17. (d) | 18. (a) | 19. (d) | 20. (b) | 21. (b) |
| 22. (c) | 23. (a) | 24. (b) | 25. (a) | 26. (d) | 27. (b) | 28. (b) |
| 29. (c) | 30. (b) | 31. (b) | 32. (c) | 33. (c) | 34. (b) | 35. (b) |
| 36. (a) | 37. (a) | 38. (c) | | | | |

## GATE Previous Year's Question

Q1. The population (N) distribution over states (n) of a diatomic molecule corresponds to **[GATE 200]**



(a) Translation (b) Vibration (c) Rotation (d) Electronic

Q2. Radiation of $10^{14}\,Hz$ falls in the region of **[GATE 2002]**

(a) Radiofrequency (b) Microwave (c) Visible (d) X-ray

Q3. The spacing between the rotational lines of the HF is $40\text{cm}^{-1}$. The corresponding spacing between the rotational lines in DF is approximately **[GATE 2002]**

(a) $20\ \text{cm}^{-1}$ (b) $30\ \text{cm}^{-1}$ (c) $60\ \text{cm}^{-1}$ (d) $7.5\ \text{cm}^{-1}$

Q4. Neglecting the mass of hydrogen $(1.0\ \text{amu})$ and deuterium $(2.0\ \text{amu})$ with respect to that of iodine $(127\ \text{amu})$, the ratio between fundamental vibrational frequencies HI and DI is **[GATE 2004]**

(a) $\frac{1}{2}$ (b) $2$ (c) $\frac{1}{\sqrt{2}}$ (d) $\sqrt{2}$

Q5. The population of $J^{th}$ rotational level $N_J$ is given by $N_j = N_0\,(2J+1)e^{-J(J+1)B/kT}$. The $J$ value of rotational level with maximum population $(J_{max})$ is given by **[GATE 2004]**

(a) $\frac{(2kT/B)-1}{\sqrt{2}}$ (b) $\frac{\sqrt{2kT/B-1}}{2}$ (c) $\frac{kT}{B}$ (d) $\frac{B}{kT}$

Q6. Require matching of items of **column-I** with the appropriate items in **column-II**. Choose the correct one form the alternate (a), (b), (c) and (d) **[GATE 2005]**

| **Column-I**<br>**Spectral Technique** | **Column-II**<br>**Selection Rule** |
|---|---|
| **P.** Rotational transition | **I.** $\Delta v = \pm 1$ |
| **Q.** Vibrational transition | **II.** $\Delta J = 0$ |
| **R.** Electronic transition in atoms | **III.** $\Delta J = \pm 1$ |
| **S.** Molecular ensemble | **IV.** $\Delta l = \pm 1$ |
| | **V.** $\Delta m_j = \pm 1$ |
| | **VI.** $\Delta v = 0$ |
| | **VII.** $\Delta l = 0$ |

(a) P-I, Q-VI, R-VII, S-V (b) P-II, Q-I, R-IV, S-V
(c) P-III, Q-I, R-IV, S-V (d) P-I, Q-VI, R-VII, S-V

Q7. The zero-point energy of the vibration of $^{35}Cl_2$ mimicking oscillator with a force constant $k = 2293.8\ Nm^{-1}$ is **[GATE 2006]**

(a) $10.5 \times 10^{-21} J$ (b) $14.8 \times 10^{-21} J$ (c) $20 \times 10^{-21} J$ (d) $29.6 \times 10^{-21} J$

Q8. The selection rules for the appearance, of P branch in the rotational-vibrational absorption spectra of a diatomic molecule within rigid rotor-harmonic oscillator model are **[GATE 2007]**

(a) $\Delta v = \pm 1$ and $\Delta J = \pm 1$ (b) $\Delta v = +1$ and $\Delta J = +1$

(c) $\Delta v = +1$ and $\Delta J = -1$ (d) $\Delta v = -1$ and $\Delta J = -1$

Q9. The $J=0 \rightarrow 1$ rotational transition for $^{1}H^{79}Br$ occurs at $500.72 GHz$ Assuming the molecule to be a rigid rotor, the $J = 3 \rightarrow 4$ transition occurs at **[GATE 2007]**

(a) $50.1\ cm^{-1}$ (b) $66.8\ cm^{-1}$ (c) $16.7 cm^{-1}$ (d) $83.5 cm^{-1}$

Q10. The rotational constant for $CO$ in the ground and the first excited vibrational states are $1.9$ and $1.6\ cm^{-1}$, respectively. The % change in the internuclear distance due to vibrational excitation is

(a) 9 (b) 30 (c) 16 (d) 0 **[GATE 2008]**

**Linked Answer Type Q.11 and Q.12**

The infrared spectrum of a diatomic molecule exhibits transition at $2144, 4262$ and $6354\ cm^{-1}$ corresponding to excitations form the ground state to the first, second and, third vibration states respectively

Q11. The fundamental transition $\left(cm^{-1}\right)$ of the diatomic molecule is at **[GATE 2008]**

(a) 2157 (b) 2170 (c) 2183 (d) 2196

Q12. The anharmonicity constant $\left(cm^{-1}\right)$ of the diatomic molecule is **[GATE 2008]**

(a) 0.018 (b) 0.012 (c) 0.006 (d) 0.003

Q13. The total number of ways in which two nonidentical spin $-1/2$ particles can be oriented relative to a constant magnetic field is: **[GATE 2008]**

(a) 1 (b) 2 (c) 3 (d) 4

Q14. The rotational Raman spectrum of $^{19}F_2$ shows a series of Stokes lines at $19230.769\ cm^{-1}$, $19227.238\ cm^{-1}$ and $19223.707\ cm^{-1}$. The rotational constant for $^{19}F_2$ in $GHz$ is: **[GATE 2009]**

(a) $26.484$ (b) $52.968$ (c) $105.936$ (d) $3.531$

Q15. The most populated rotational state for $HCl\left(B = 8.5 cm^{-1}\right)$ at $300K$ is **[GATE 2010]**

(a) $2$ (b) $3$ (c) $5$ (d) $7$

Q16. The ratio of life times of two states that gives rise to line width of $1.0\ cm^{-1}$ and $0.2\ cm^{-1}$ respectively is

(a) $1:2$ (b) $1:5$ (c) $2:1$ (d) $5:1$

**Common Data for Q.17 and Q.18**

A hypothetical molecule XY has the following properties

Reduced mass: $2\times10^{-26}$ kg X-Y bond length : 100 pm

Force constant of the bond: $8\times10^{2}$ N.m$^{-1}$

Q17. The frequency of radiation (in $cm^{-1}$ units) required to vibrationally excite the molecule from $v = 0$ to $v = 1$ state is **[GATE 2011]**

(a) $3184.8$ (b) $2123.2$ (c) $1061.6$ (d) $840.0$

Q18. The frequency of radiation (in $cm^{-1}$ units) required to rotationally excite the molecule from $J=0$ to $J=1$ state is **[GATE 2011]**

(a) $1.4$ (b) $2.8$ (c) $3.2$ (d) $3.6$

**Statement For Linked Answer for Q.19 and Q.20**

A $20491\ cm^{-1}$ laser line was used to excite oxygen molecules (made of $^{16}O$ only) to obtain the rotational Raman spectrum. The resulting rotational Raman spectrum of oxygen molecule has the first Stokes line at $20479\ cm^{-1}$

Q19. The rotational constant (usually denoted as B) for the oxygen molecule is **[GATE 2012]**

(a) $1.2\ cm^{-1}$ (b) $2.0\ cm^{-1}$ (c) $3.0\ cm^{-1}$ (d) $6.0\ cm^{-1}$

Q20. The next rotational Stokes line is expected at **[GATE 2012]**

(a) $20467\ \text{cm}^{-1}$ (b) $20469\ \text{cm}^{-1}$ (c) $20471\ \text{cm}^{-1}$ (d) $20475\ \text{cm}^{-1}$

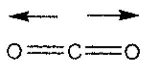
Q21. The infrared spectrum of HCl gas shows an absorption band centered at $2885\ \text{cm}^{-1}$ .The zero point energy of HCl molecule under harmonic oscillator approximation is: **[GATE 2013]**

(a) $2.8665\times10^{-22}\text{J}$ (b) $2.8665\times10^{-20}\text{J}$ (c) $5.7330\times10^{-2}\text{J}$ (d) $5.7330\times10^{-20}\text{J}$

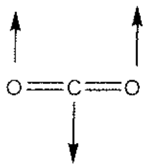
Q22. The ratio of molecules distributed between two states is $9.22\times10^{6}$ at $300\text{K}$ . The difference in energy (in $\text{kJmol}^{-1}$ ) of the two states is ——————— **[GATE 2014]**

Q23. Consider a two-state system at thermal equilibrium with equal degeneracy where the excited state is higher in energy than the ground state by $0.1\,\text{eV}$ . The ratio of the population of the excited state to that of the ground state, at temperature for which $k_BT = 0.05\text{eV}$, is ——————— **[GATE 2016]**

Q24. Of the vibrational modes given below, the IR active mode(s) is(are) **[GATE 2016]**

(i) 

(ii) 

(iii) 

(a) (ii) only (b) (iii) only (c) (i) and (ii) (d) (ii) and (iii)

Q25. The lowest energy of a quantum mechanical one-dimensional simple harmonic oscillator is $300\ \text{cm}^{-1}$ . The energy (in $\text{cm}^{-1}$ ) of the next higher level is ——————— **[GATE 2017]**

Q26. For a diatomic vibrating rotor, in vibrational level $\text{v} = 3$ and rotational level $J$, the sum of the rotational and vibrational energies is $11493.6\ \text{cm}^{-}$ . Its equilibrium oscillator frequency is $2998.3\ \text{cm}^{-1}$, anharmonicity constant is $0.0124$ and rotational constant under rigid rotor approximation is $9.716\ \text{cm}^{-1}$ . The value of $J$ is ——————— **[GATE 2018]**

(Upto nearest integer)

Q27. The spacing between the two adjacent lines of the microwave spectrum of $\text{H}^{35}\text{Cl}$, is $6.35\times1011\text{Hz}$ , given that bond length $\text{D}^{35}\text{Cl}$ is $5\%$ greater than of $\text{H}^{35}\text{Cl}$ the corresponding spacing for $\text{D}^{35}\text{Cl}$ ———————

$\times10^{11}\text{Hz}$ . (Upto two decimal places) **[GATE 2018]**

## Answer Key

1. (c) 2. (c) 3. (a) 4. (d) 5. (b) 6. (c) 7. (b)

8. (c) 9. (b) 10. (a) 11. (b) 12. (c) 13. (c) 14. (a)

15. (b) 16. (b) 17. (c) 18. (b) 19. (a) 20. (b) 21. (b)

22. (38 to 42) 23. (0.13 to 0.14) 24. (d) 25. (899 to 901)

26. (12) 27. (2.95)

## TIFR Previous Year's Question

Q1. The stretching frequency of the O-H is about $3600\ \text{cm}^{-1}$. Compared to that, the stretching frequency of O-D and S-H bonds are very similar and about $2500\ \text{cm}^{-1}$. What can you conclude from these data **[TIFR 2010]**

(a) The electronic structure of O-D and O-H are same, and that S-H is different

(b) The force constant of the bond O-D and O-H is same.

(c) S-His a weaker bond than O-H or O-D bond

(d) All of these above

Q2. Read the following two statements carefully.

1. The changes in total angular momentum that occurs when a diatomic molecule (i. e. a rigid rotor) change rotational level from $J=2$ to $J=3$ is the same as the change in total angular momentum the occurs when an electron on a H atom changes from a d to an f orbital, i. e. form $l=2$ to $l=3$
2. The change in energy that occurs when a diatomic molecule (i. e. rigid rotor) changes rotational level from $J=2$ to $J=3$ is the same as the change in energy that occurs when a electron on a H atom changes from a d to an f orbitals i. e. from $l=2$ to $l=3$

Based on the above, which of the following is the correct statements **[TIFR 2010]**

(a) Both statement 1 and 2 are true (b) Both statement 1 and 2 are false

(c) statements1 is true, statement 2 is false (d) Statement 1 is false, and statement 2 is true

Q3. The vibrational Raman effect, a considerably weak scattering phenomena, was first reported by Late Sir CV Raman in 1928. The intensity of the individual vibrational resonances observed in a Raman spectrum is proportional to **[TIFR 2012]**

(a) Number of molecules (b) Polarizibility of the bond

(c) Wavelength of radiation used (d) All of the above

Q4. Rotational energy diatomic molecules is given by $E_{rot}=J(J+1)hB_e$, where $E_{rot}$ is in Joules. If the rotational constant for $H_2$ molecule is given as $B_e=1.8324\times10^{12}\,\text{Hz}$, the rotational period of the $H_2$ molecule in $J=10$ level will be **[TIFR 2012]**

(a) $1.33\times10^{-19}$ sec (b) $5.0\times10^{-15}$ sec (c) $5.46\times10^{-13}$ sec (d) $7.39\times10^{-7}$ sec

Q5. The transition probability for spontaneous emission form state $m$ to state $n$ is given by an expression

$$A_{m\to n}=\left(\frac{64\pi^4\upsilon_{mn}^3}{3hc^3}\right).\left(\left|\langle m|\hat{d}|n\rangle\right)\right)$$

Where $V_{nm}$ is the frequency of transition, and the term in the parenthesis is the transition dipole. Assuming that magnitude of the transition dipole is same for all type of transitions, arrange the average lifetimes for the electronic, vibrational transitions in the proper order. **[TIFR 2012]**

(a) electronic $<$ vibrational $<$ rotational (b) vibrational $<$ rotational $<$ electronic

(c) rotational $<$ vibrational $<$ electronic (d) electronic $<$ rotational $\approx$ vibrational

Q6. Consider a classical harmonic oscillator with a mass 'm' and a force constant 'k' oscillating with a frequency 'v' . Which of the following statements is NOT true for this system ? **[TIFR 2013]**

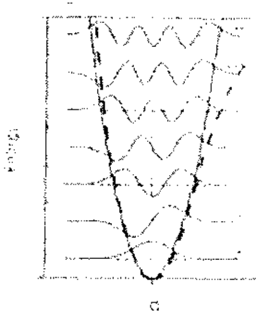
(a) 'v' increase if 'm' decrease

(b) The oscillator is most likely to be found at its equilibrium position

(c) The acceleration is maximum at its turning points

(d) 'v' does not depend on how large the amplitude of the oscillation is

Q7. Shown below in solid-line in the harmonic potential of a quantum oscillator for a diatomic molecule. If the harmonic potential is suddenly transformed into Morse potential shown in dashed-line how would the zero point energy shape of wavefunction change? **[TIFR 2013]**



(a) Zero-point energy remains the same and wavefunction do not change
(b) Zero-point energy remains the same but wavefunction reflects a change on the high Qside
(c) Zero-point energy changes and wavefunction reflects a change on the high Q side.
(d) Potential never reflect any change in the shape of the wavefunction.

Q8. Which of the following statements is/are true **[TIFR 2014]**

(i) HCl absorbs IR radiation (ii) $CO_2$ absorbs IR radiation

(iii) H atom absorbs IR radiation (iv) H atoms UV -vis and microwave radiation

(a) (i) only (b) (i) and (ii) only

(c) (i),(ii) and (iii) only (d) (i),(ii),(iii) and (iv)

Q9. $N_2$ does not shows pure vibrational spectra because **[TIFR 2014]**

(a) triplet 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

Q10. Raman scattering is often seen overlapping with fluorescence emanating form the sample. However, fundamentally Raman process is different form fluorescence. This is because **[TIFR 2014]**

(a) Raman scattering is a two – photon process and fluorescence is not

(b) Raman process is a scattering process while fluorescence is not

(c) Raman process need not be stoke shifted

(d) All of the above

Q11. How many normal modes does the $CO_2$ molecule have? What if the C and the O atoms were constant to move in one dimension? **[TIFR 2015]**

(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 $CO_2$

Q12. Which of the following statements are true? **[TIFR 2015]**

(i) For a harmonic oscillattor potential, the spacing between adjacent energy levels remain constant with increasing the quantum number.

(ii) For a Morce oscillator potential, the spacing between adjacent energy levels increase with increasing the vibrational quantum number.

(iii) Harmonic oscillators are be used to explain the bond dissociation

(iv) Morse oscillator can be used to explain the vibration of molecule.

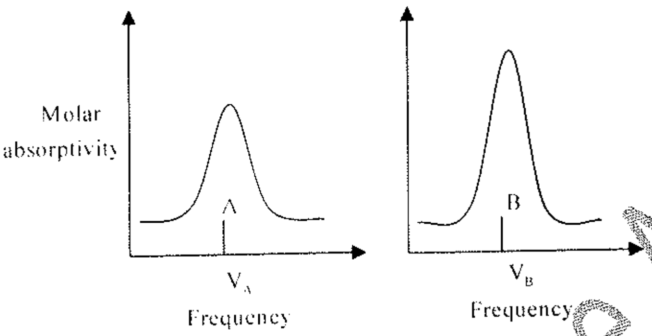
(a) i,ii and iii only(b) i and iv only (c) i,ii and iv only (d) i,ii,iii and iv only

Q13. For a harmonic oscillator in its ground state i. e. $v = 0$ states, the energy is given by $E = \frac{1}{2}hv$ where v is the vibrational frequency. This is due to its **[TIFR 2015]**

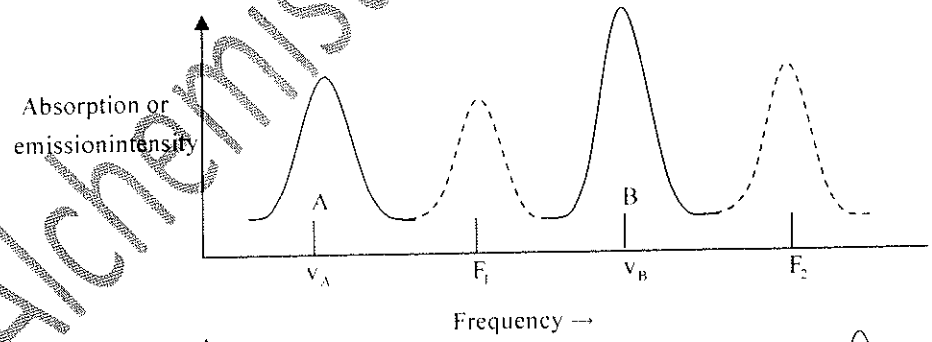
(a) Kinetic energy (b) Potential energy

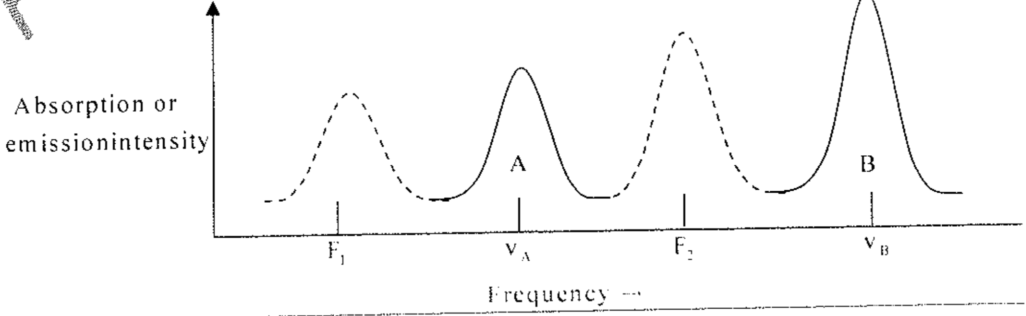
(c) Sum of kinetic and potential energy (d) Heat of formation

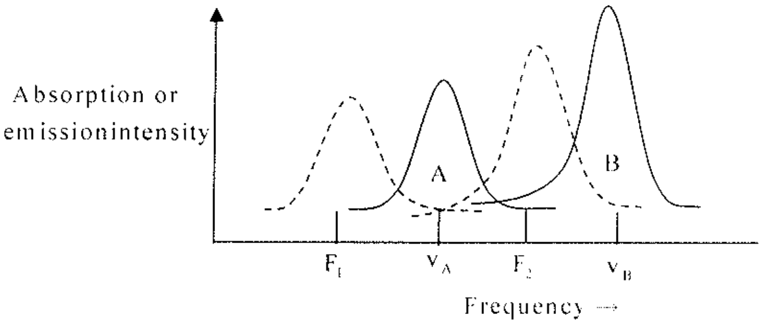
Q14. The electronic absorption spectra or two species A and B are shown below **[TIFR 2015]**

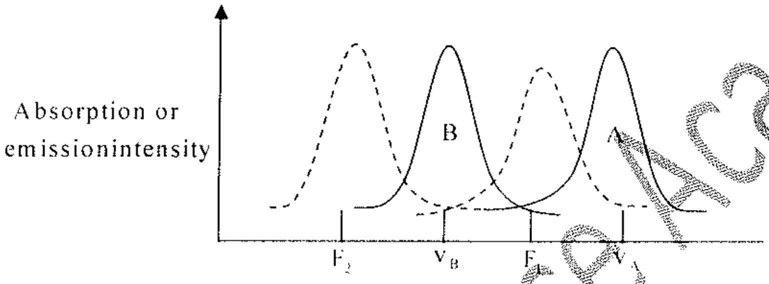


In a solution, these two species are dissolved, and they are moving freely. Using a tunable laser, when the solution is excited at $V_A$, a single fluorescence band is seen around frequency $F_1$. When the laser frequency is changed to $V_B$, two fluorescence band are seen around frequencies $F_1$ and $F_2$. Which of the following figures can qualitatively describe the correct relative position of the frequencies $v_A, v_B, F_1$ and $F_2$ ? The continuous line shows absorption and the dashed line shows fluorescence emission spectra.









Q15. Far infrared and microwave radiation is useful in studying the following process **[TIFR 2016]**

(a) Transition of inner electrons of atoms

(b) Transition od outer (or valence) electrons in atoms or molecules

(c) Changes in vibrational-rotational states of molecules

(d) Changes in molecular rotational only

Q16. Isotopic substitution is an often-used procedure in assigning vibrational spectroscopic features but the difference in isotopic masses of the vibrating atoms has to be sufficiently large to make the vibrational shift observable. In a double isotopic replacement experiment, a proline with a $^{13}C = ^{18}O$ carbonyl group is inserted in the middle of the polypeptide using molecular recombinant techniques. Given that the naturally found prolineth e $^{12}C = ^{16}O$ group exhibits a narrow vibrational feature at $11.711 cm^{-1}$, what is the shift of the carbonyl stretching vibration for the $^{13}C = ^{18}O$ prolineisotomer.

Assume:

(A) The force constant for different isotopes can be consider identical.

(B) The isotopic changes in the carbonyl group will have little effect on the vibrations of other atoms in proline

(a) $80 cm^{-1}$ (b) $165 cm^{-1}$ (c) $85 cm^{-1}$ (d) $42.5 cm^{-1}$

Q17. In a rotational microwave spectrum of $C^{12}O^{16}$ lines were equally spaced by $3.663cm^{-1}$. In a rotational Raman spectrum of $N_2$ (normal isotope) the lines where equally spaced by $8.04cm^{-1}$. Assuming that the force constant for the two molecules is inversely proportional to their bond lengths, the ratio of the vibrational frequency of CO to that of $N_2$ will be **[TIFR 2017]**

(a) $0.8368$ (b) $0.9952$ (c) $1.0258$ (d) $1.2198$

Q18. Suppose you are carrying out an experiment measuring the Raman spectrum of $N_2$ gas in the outdoor air. Where would you find a higher strength of the anti-Stokes line **[TIFR 2017]**

(a) In Kanyakumari

(b) On top of Mt. Everest

(c) The strength will be the same in both the places

(d) Nitrogen would not have an anti-Stokes Raman line

Q19. The fully symmetric $C-H$ stretching mode $(a_1)$ of $CH_4$ was detected to be at $3025cm^{-1}$. The $C-H$ bending mode $(t_2)$ on the other has was detected to be at $1380cm^{-1}$. If complete H/D exchange lebeling was done to produces the molecule $CD_4$, and the frequency ratio $R_D$ is defined as $=[V_{bend}V_{stretch}]$ for $CD_4 R_H=[V_{bend}/V_{stretch}]$ for ethane; which of the following statements is TRUE about $R_H ? R_D$ an dthe vibrational technique used for detection: **[TIFR 2018]**

(a) $R_H/R_D=1.4$ while IR spectrum can be used to detect both the symmetric stretch and the bending mode

(b) $R_H/R_D=1.0$ while Raman spectroscopy can be used to detect both the symmetric stretch and the bending mode

(c) $R_H/R_D=1.0$ while IR can detect the symmetric stretch stretch and Raman the bending mode

(d) $R_H/R_D=1.4$ while Raman can detect the symmetric stretch and IR the bending mode.

Q20. The rotational constant for a diatomic molecule is $1.9225cm^{-1}$ In general (Within the rigid rotor approximation), at $T=600K$, for a rotation state with maximum population $(J_{max})$ and the position of maximum intensity of pure rotational absorption spectrum $(I_{max})$, which of the following holds true **[TIFR 2018]**

(a) $J_{max}=7$, while $I_{max}$ position is near transitions originating form $J=7$

(b) $J_{max}=10$ while $I_{max}$ position is near transition originating from $J=7$

(c) $J_{max}=7$, while $I_{max}$ position cannot be determined from this information alone

(d) $J_{max}=10$, while $I_{max}$ position cannot be determined form this information alone.

## Answer Key

1. (b)
2. (c)
3. (d)
4. (b)
5. (a)
6. (b)
7. (d)
8. (d)
9. (b)
10. (d)
11. (d)
12. (b)
13. (c)
14. (c)
15. (d)
16. (a)
17. (b)
18. (a)
19. (b)
20. (d)

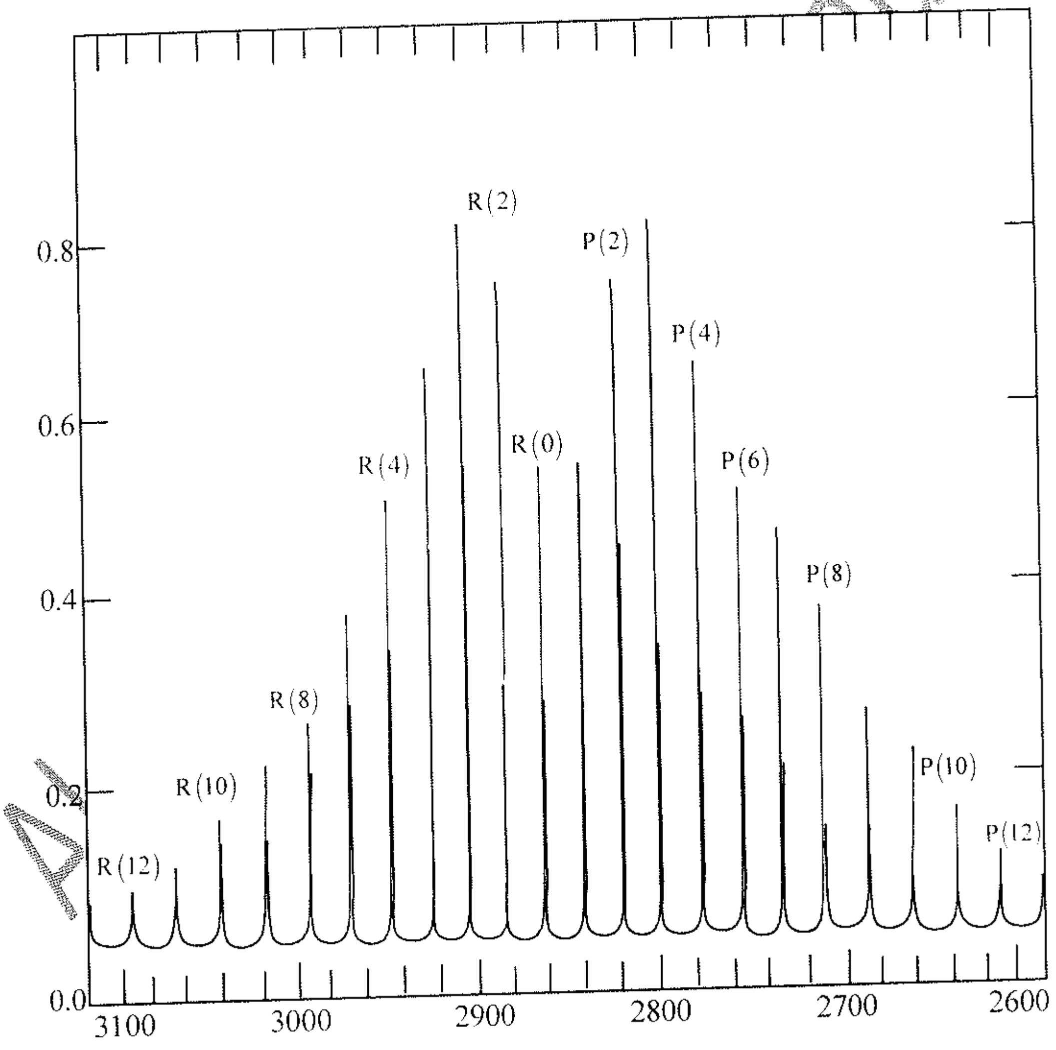
## Other Examination Previous Year's Question

Q1. The lines in the microwave spectrum of $^{1}H^{127}I$ are separated by A $cm^{-1}$. The lines in the microwave spectrum of $^{2}H^{127}I$ will be separated by

(a) $A/4$ (b) $A/2$ (c) $A/\sqrt{2}$ (d) $A$

**Common Information for Q.2 and Q.3.**

Shown below is a vibrational – rotational spectrum for a diatomic molecule with reduced mass $=10^{-26}$ kg recorded at temperature $T$.



Q2. Moment of inertia $\left(\text{kgm}^2\right)$ is:

(a) $1.0\times10^{-46}$ (b) $1.2\times10^{-47}$ (c) $5.0\times10^{-47}$ (d) $2.5\times10^{-47}$

Q3. Determine the correctness or otherwise Assertion $[\text{a}]$ and Reason $[\text{r}]$.

**Assertion** $[\text{a}]$: Usually symmetric vibrations give rise to intense Raman lines. Non-symmetric ones are usually weak and sometimes not observed.

**Reason** $[\text{r}]$: Change I dipole is the highest during symmetric vibrations than the change during the non-symmetric ones.

(a)**Both** $[\text{a}]$ and $[\text{r}]$ are the true $[\text{r}]$ is the correct reason for $[\text{a}]$.

(b)**Both** $[\text{a}]$ and $[\text{r}]$ are true but $[\text{r}]$ is not the correct reason for $[\text{a}]$

(c) **Both** $[\text{a}]$ and $[\text{r}]$ are false

(d) $[\text{a}]$ is true but $[\text{r}]$ is false

Q4. The force constant $\left(\text{in Nm}^{-1}\right)$ is:

(a) $2.9\times10^{-3}$ (b) $5.8\times10^{3}$ (c) $1.2\times10^{4}$ (d) $5.8\times10^{4}$

Q5. Normal mode of vibration for the molecule $C_2H_4$ is

(a) 18 (b)15 (c)12 (d) 6

Q6. The vibrational-rotational energy of a diatomic may be written as (where $\nu$ is the frequency of vibration, and $I$ is the moment of inertia of the molecules).

(a) $\left(n+1/2\right)h\nu+\frac{h^2}{2I}J\left(J+1\right), n=1,2,3...J$ and $= 0,1,2......$

(b) $\left(n+1/2\right)h\nu+\frac{h^2}{2I}J\left(J+1\right), n=0,1,2,3...$ and $J=0,1,2$

(c) $\left(n+1/2\right)h\nu+\frac{\hbar^2}{2I}M^2, n=1,2,3.......$ and $M=0,\pm1,\pm2,\pm3........$

(d) $\left(n+1/2\right)h\nu+\frac{\hbar^2}{2I}M^2, n=0,1,2,3.......$ and $M=0,1,2,3.....$

Q7. Given that the rotational energy $BJ(J+1)$, where the rotational constant has a value $B = 0.2\text{cm}^{-1}$ and kT is $209\text{cm}^{-1}$ the approximate ratio of population of two rotational states with $J = 10$ and $20$ are

(a) $1:2$ (b) $2:1$ (c) $19:27$ (d) $21:41$

Q8. The moment of inertia for HCl gas can be determined form its microwave spectrum. Which property of the HCl molecule may be obtained form the moment of inertia?

(a) the vibrational frequency (b) the force constant

(c) the bond strength (d) the bond length

Q9. A wave of length $10\ \text{nm}$ is traveling at a speed of $10^6 \text{m/s}$. The frequency of the wave is,

(a) $3\times10^{16}\text{Hz}$ (b) $10^{14}\text{Hz}$ (c) $3\text{Hz}$ (d) $3\times10^{14}\text{Hz}$

Q10. The selection rules for the allowed rotation Raman lines is

(a) $\Delta J = 0, \pm 2$ (b) $\Delta J = \pm 1$ (c) $\Delta J = 0$ (d) $\Delta J = 0, \pm 1$ and $\pm 2$

Q11. Replacement of hydrogen by deuterium atom bond to a heavy atom X in a polyatomic molecules would reduce the vibrational frequency of the...X-Y stretching by a factor of

(a) $2$ (b) $\sqrt{2}$ (c) $4$ (d) $1.3$

Q12. The first line in the rotational Raman spectra of a diatomic molecules appears with a stock shift of $12\ \text{cm}^{-1}$. The Stoke shift for the second line is:

(a) $36\ \text{cm}^{-1}$ (b) $24\ \text{cm}^{-1}$ (c) $18\ \text{cm}^{-1}$ (d) $20\ \text{cm}^{-1}$

Q13. The $R$ branch in the vibrational spectra of AX exhibits a set of equally spaced lines with a separation of $10\text{cm}^{-1}$. The rotational constant of AX is:

(a) $10\ \text{cm}^{-1}$ (b) $20\ \text{cm}^{-1}$ (c) $5\ \text{cm}^{-1}$ (d) $15\ \text{cm}^{-1}$

Q14. Overtones are observed in the vibrational spectra of diatomic molecules when

(a) Anharmonicity is large

(b) Anharmonicity is absent

(c) Vibrational and rotational modes are coupled

(d) An alternating electric field is applied.

Q15. The selection rule four observing rotational Raman spectrum is:

(a) $\Delta J = \pm 1$ (b) $\Delta J = \pm 2$ (c) $\Delta J = 0$ (d) $\Delta J = \pm 3$

Q16. The wavelength of light emitted when electron falls form the $n=50$ orbits to the $n=49$ orbits of H - atoms, is

(a) 55nm (b) 0.55cm (c) $0.55\overset{0}{A}$ (d) 55n

Q17. Which of the following molecules has the lowest vibrational stretching frequency?

(a) $^{4}H^{35}Cl$ (b) $^{2}H^{35}Cl$ (c) $^{4}H^{36}Cl$ (d) $^{4}H^{37}Cl$

Q18. A radiation which has an energy of $N\ 50\ kJ\ Mol^{-1}$ falls in the following region of the electromagnetic spectrum.

(a) infrared (b) visible (c) ultraviolet (d) microwave

Q19. The microwave spectrum of a molecule yields three rotational constants. The molecule is

(a) Prolate symmetric top (b) Spherical top

(c) Asymmetric top (d) Oblate symmetric top

Q20. A certain molecule can be treated as having only a doubly degenerate state lying at $360\ cm^{-1}$ above the nondegenerate ground state. The approximate temperature $(K)$ at which $15\%$ of the molecules will be in the upper state is:

(a) 500 (b) 150 (c) 200 (d) 300

Q21. When $^{14}N_2$ (with rotational constant of $1.99\ cm^{-1}$) is exposed to $340\ nm$ light, then the strokes and anti-stokes lines for the molecule is second rotational state can be observed at

(a) $29412\ cm^{-1}$ and $29410\ cm^{-1}$ (b) $340.3\ nm$ and $339.9\ nm$

(c) $14779.9\ cm^{-1}$ and $58529.9\ cm^{-1}$ (d) $29384\ cm^{-1}$ and $29424\ cm^{-1}$

Q22. The magnitude of the nuclear spin angular momentum of a nuclei $\sqrt{15/2h}$ units. The value of I is

(a) $5/2$ (b) $1/2$ (c) $I$ (d) $3/2$

Q23. The rotational constant $(B)$ of $H^{35}Cl, H^{37}Cl$ and $D^{35}Cl$ follows the order

(a) $H^{35}Cl > D^{35}Cl > H^{37}Cl$ (b) $H^{35}Cl > H^{37}Cl > D^{35}Cl$

(c) $D^{35}Cl > H^{35}Cl > H^{37}Cl$ (d) $H^{37}Cl > H^{35}Cl > D^{35}Cl$

Q24. At a given temperature, for a rigid rotor, the probability that the system is in the rotational state $J=0$ is $0.6$, in state $J=1$ is $0.3$, and $0.1$ in $J=2$. The energy in a rotational state J is given by $J(J+1)B$, where B is the rotational constant. The average of the rotor at the give temperature is

(a) $-6.0B$ (b) $1.2B$ (c) $3.6B$ (d) $4.8B$

Q25. The fundamental vibrational frequency V of a homonuclear diatomic molecule with atomic Mass $m$ and force constant $k$ is

(a) $v=\frac{1}{2\pi}\sqrt{\frac{k}{m}}$ (b) $v=\frac{1}{v}\sqrt{\frac{2k}{m}}$ (c) $v=\frac{1}{2\pi}\sqrt{\frac{k}{2m}}$ (d) $v=\frac{2}{2\pi}\sqrt{\frac{k}{m}}$

Q26. An anharmonic diatomic oscillator has a frequency of $3000\ cm^{-1}$ and dimensionless anharmonicity of $1/30$. The diatoms is made to dissociate by supplying energy equal To the potential well. The minimum relative kinetic energy of the ejected atom will be

(a) $1400\ cm^{-1}$ (b) $1450\ cm^{-1}$ (c) $1475\ cm^{-1}$ (d) $1500\ cm^{-1}$

Q27. The moment of inertia of CO molecules is $1.46\times10^{-46}kg.m^2$. The angular velocity in the $J=1$ energy level of CO molecules is

(a) $9.14\times10^{11}rad.sec^{-1}$ (b) $10.20\times10^{11}rad.sec^{-1}$

(c) $11.44\times10^{11}rad.sec^{-1}$ (d) $12.86\times10^{11}rad.sec^{-1}$

Q28. The optimized variational wavefunction 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.

Q29. For a simple diatomic molecules, the functional form of the potential energy curve can be expressed (with usual terms) as

(a) $V(r)=D_e\left[1+e^{-a(r-r_e)^2}\right]$ (b) $V(r)=D_e\left[1-e^{-a(r-r_e)^2}\right]$

(c) $V(r)=-D_e\left[e^{-a(r-r_e)^2}-1\right]$ (d) $V(r)=D_e\left[1-e^{a\left(1-e^{(r-r_e)^2}\right)}\right]$

Q30. The mathematical form of transition dipole moment (with usual terms) for an optical transition form initial state $(i)$ to final state $(f)$ for visible radiation interaction with matter is given by

(a) $\langle \psi_f | M | \psi_i \rangle$ (b) $\langle \psi_f | \mu | \psi_i \rangle$ (c) $\langle \psi_f | r.\mu | \psi_i \rangle$ (d) $\langle \psi_i | \mu | \psi_f \rangle$

Q31. The bond length for $H^9F$ is $91.68 \times 10^{-12}$ m . Where does the axis of rotation intersect the molecular axes?

(a) Exactly in between F and H atoms (b) Axis of rotational is close to F

(c) Axis of rotation is close to H (d) Far away to the right of F

Q32 The number of IR active bands in $H_2O$ molecules is

(a) 2 (b) 3 (c)4 (d) 1

Q33. The energy of rotational level with $J = 10$, in wave number $(cm^{-1})$ unit is

(a) 2B (b) 110B (c)220B (d) 10B

Q34. The molecule which shows some common lines in the IR and Raman spectra is

(a) $CO_2$ (b) $CS_2$ (c) $N_2O$ (d) $H_2$

Q35. Which of the following molecules has a microwave spectra?

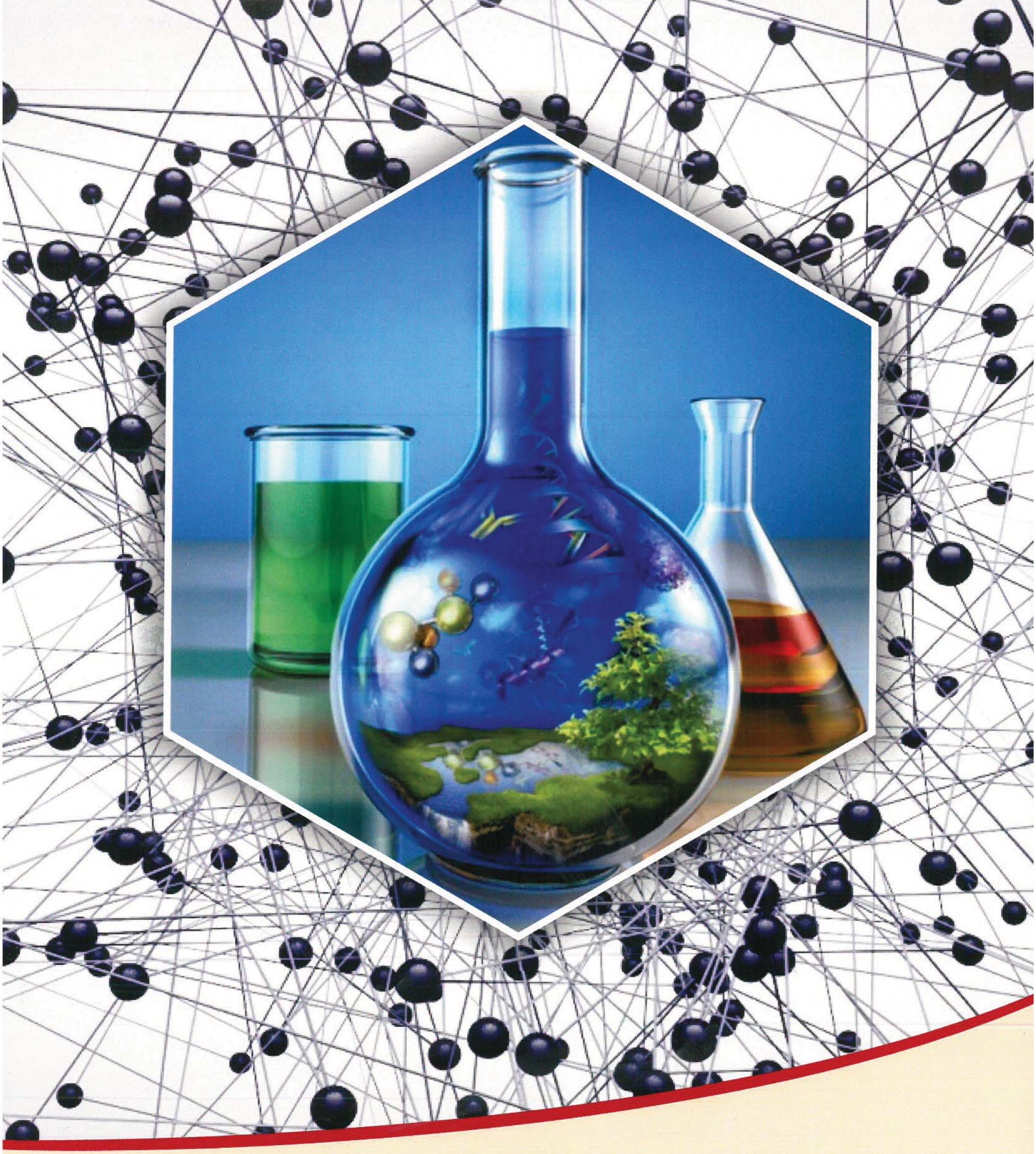
(a) $CO_2$ (b) $CH_2 = CH_2$ (c) $C_6H_6$ (d) OCS

Q36. Which of the following molecules is infrared inactive?

(a) NO (b) $N_2O$ (c) $H_2$ (d) $CH_4$

## Answer Key

1. (b) 2. (b) 3. (*) 4. (a) 5. (c) 6. (c) 7. (d)
8. (d) 9. (b) 10. (a) 11. (b) 12. (d) 13. (c) 14. (a)
15. (b) 16. (b) 17. (c) 18. (a) 19. (c) 20. (c) 21.(d)
22. (d) 23. (b) 24. (b) 25. (b) 26. (c) 27. (b) 28. (a)
29. (b) 30. (b) 31. (b) 32. (b) 33. (b) 34. (c) 35. (d)
36. (c)



# ALCHEMIST SCIENCE ACADEMY

28-/A, Jia Sarai, Hauz Khas, New Delhi-16 • Ph. : 011-26511021, 8285787633, 9582285416, 9149049297
www.csirnetalchemist.com • alchemistscienceacademy@gmail.com