1. (a) Calculate the number of translational, rotational and vibrational degrees of freedom for

(i) CO_2 (ii) H_2O (iii) Benzene (iv) CH_4 (v) HCN

(b) The $^1H^{35}C1$ molecule shows pure rotational lines at the following frequencies (cm^{-1}) 20.7, 41.5, 62.0, 83.0, 103.8. Calculate the bond distance of HC1. ($m_H = 1.673 \times 10^{-27}$kg, $m_{Cl} = 58.06 \times 10^{-27}$kg).

(c) Draw the different modes of vibration in the following two polyatomic molecules : water and carbon dioxide. (5,5,5)

2. (a) What is the effect on the microwave spectrum of $C^{16}O$ if ^{16}O is substituted by ^{18}O?

(b) Arrange the following groups in increasing order of their absorption frequencies : Give justification

(i) CF, CC1, CBr, CH

(ii) C-C, C=C, C≡C

(c) The force constant for $^1H^{19}F$ is 966 Nm^{-1}. Calculate :

(i) The zero-point vibrational energy of this molecule when it follows harmonic motion.

(ii) The frequency of the electromagnetic radiation to excite this molecule from the ground state to the first excited state. (5,5,5)

3. (a) What is Raman effect? Explain the origin of Stokes and Anti-Stokes line.

(b) A molecule XY_2 has the following IR and vibrational Raman spectral data :

$\bar{\upsilon}$ (cm^{-1})	IR	Raman
1243	Inactive	Active
2920	Active (PR)	Inactive
786	Active (PQR)	Inactive

Giving proper explanation, arrive at the geometry of the molecule. Assign the wave numbers to specific vibrations.

(c) What is TMS? Why is it used as a standard in NMR spectroscopy? (5,5,5)

4. (a) What is the selection rule for Raman rotational spectrum of diatomic molecules? Show that the Raman lines will appear at wavenumbers given by

$$\bar{\upsilon} = \bar{\upsilon_0} + B\,(4J + 6)$$

where $\bar{\upsilon_0}$ is the wavenumber corresponding to the Rayleigh line.

(b) What is the difference between spin-spin relaxation and spin-lattice relaxation?

(c) Calculate the precessional frequency of a proton in a magnetic field of strength of 2.349 T. (5,5,5)

P.T.O.

5. (a) Given that the spin quantum numbers of $^{12}C6$, $^{1}H_1$, and $^{2}D_1$ are zero, half, and one, respectively, how many different energy states do these nuclei have in a magnetic field? Which of these atoms will show peak in the NMR spectra?

   (b) What are the fundamental requirement for a molecule to show :

   (i) Rotational

   (ii) IR

   (iii) Raman and

   (iv) NMR spectra

   (c) The fundamental and the first overtone transitions of HBr are centered at 2560 and 5028 cm^{-1} respectively. Calculate the anharmonicity constant and the force constant of HBr. (5,5,5)

6. Write short notes on any **three** of the following :

   (a) Scanning Electron Microscope

   (b) Overtones and Combination Bands

   (c) Chemical shift in NMR spectroscopy

   (d) Intensity of spectral lines/bands (5,5,5)

[This question paper contains 4 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 9917 **K**

Unique Paper Code : 2173010043

Name of the Paper : DSE: Molecular Spectroscopy & Structural Analysis

Name of the Course : **B.Sc. (Prog.) Physical Sciences/Life Sciences**

Semester : VII

Duration : 2 Hours Maximum Marks : 60

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Answer **four** questions in all.
3. Attempt **all** parts of a question together.
4. Use of scientific calculators is allowed.

Physical Constants

Planck's constant 6.626×10^{-34} *Js*
Velocity of light 3×10^{8} *m/s*
Atomic mass unit 1.661×10^{-27} *kg*
Avagadro's number 6.023×10^{23} mol^{-1}
Mass of electron 9.109×10^{-31} *kg*