Registration No: | | | | | | | | | | |

Total Number of Pages : 02

Course: M.Sc.I
Sub Code: FCYE704

7th Semester Regular Examination: 2024–25
SUBJECT: Molecular Spectroscopy
BRANCH(S): M.Sc.I (AC)
Time: 3 Hours
Max Marks: 70
Q.Code: R193
Answer Question No.1 (Part-I) which is compulsory, any five from rest (Part-II)
The figures in the right hand margin indicate marks.

Part-I

Q.1 **Answer the following questions:** **(2 x 10)**

a) Explain the Stark effects.

b) Give the ground state term symbols for an atom with the configuration $3d^4$.

c) How will the rotational spectra change when ^{12}C in $^{12}C^{16}O$ replaced by ^{13}C?

d) What do you mean by polarizability and its consequence on Raman scattering.

e) Elucidate the structure of N_2O and CO_2 from the following infrared and Raman data.

N_2O			CO_2		
$\bar{\nu}$ (cm^{-1})	Infrared	Raman	$\bar{\nu}$ (cm^{-1})	Infrared	Raman
589	Active (PQR)	Inactive	667	Active (⊥) (PQR)	Inactive
1285	Active (PR)	Active (Polarized)	1330	Inactive	Active
2224	Active (PR)	Active (Depolarized)	2349	Active (∥) (PR)	Inactive

f) Explain Koopmans' theorem.

g) What is the selection rule for pure rotational Raman spectroscopy?

h) What is the influence of nuclear spin on infrared spectrum of molecules?

i) Propose a structure for a compound with the formula C5H9ClO.
1H NMR Data: δ6.07 (1H, multiplet) alkene H, δ5.43 (1H, d) alkene H, δ5.31 (1H, d) alkene H, δ4.04 (2H, d), δ3.83 (2H, t), δ3.65 (2H, t)

j) Explain chemical shift.

Part-II

Long Answer Type Questions (Answer Any five)

Q.2 **a)** Find out the microstates and terms of the d^2- electronic configuration **(5+5)**

b) Explain the Zeeman effect using atomic spectra of Na atom.

Q.3 **a)** Derive an expression of energy for rotational spectra of rigid rotor model. **(5+5)**

b) Calculate the most populated level (J_{max}) for CO molecule at 25 °C, if the internuclear distance is 0.133 nm.

Q.4 **a)** Discuss the origin of P, Q, and R bands in vibrational-rotational spectra. **(5+5)**

b) The fundamental and first overtone of $^{1.008}H^{35.453}Cl$ molecule are centered at 2886 cm^{-1} and 5668 cm^{-1}, respectively. Evaluate the equilibrium vibration frequency, the anharmonicity constant, zero-point energy, and force constant of the molecule.

Q.5 **a)** Explain the Raman scattering on account of the quantum theory. **(5+5)**

b) A substance shows a vibrational Raman line at 456.8 nm when the incident radiation is at 433.2 nm. Calculate the wavelength for the Stokes and Anti-Stokes line for this substance when incident radiation is at 403.6 nm.

Q.6 **a)** State the principle of photoelectron spectroscopy. Discuss the photoelectron spectra of simple polyatomic molecules. **(5+5)**

b) Discuss the rotational and vibrational Raman spectroscopy.

Q.7 **a)** Discuss the mechanism of electron shielding and deshielding, and factors contributing to the magnitude of chemical shift. **(5+5)**

b) Explain the term nuclear spin-spin coupling. Why does a peak for a particular set of protons split into a multiplet with suitable example?

Q.8 **a)** Derive the relationship between Einstein's coefficients. **(5+5)**

b) Discuss the transition dipole moments and general selection rules based on symmetry ideas.