Name: **Enrolment No:**	UPES UNIVERSITY WITH A PURPOSE

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
End Semester Examination (Online Mode), Dec 2020

Course: Molecular structure: S & D methods — **Semester:** III
Program: M. Sc. Chemistry — **Time:** 3 hrs
Course Code: CHEM 8001 — **Max. Marks:** 100

SECTION - A **6 x 5 = 30 Marks**

1. Each Question will carry 5 Marks
2. Instruction: Complete the statement / Select the correct answer(s)

Q 1	(a) State which of the following molecules have pure vibrational absorption spectra? N_2, CO_2, OCS, H_2O, $CH_2{=}CH_2$ (b) Justification for the choice of correct answer:_____	CO1
Q 2	(a) The gross selection rule of rotational and Raman spectra are _____ (b) The selection rule for CO2 molecule in case of perpendicular vibration is (i) $\Delta v = \pm 1, \Delta J = \pm 1$ (ii) $\Delta v = \pm 1, \Delta J = 0, \pm 1$ (iii) $\Delta v = 0, \pm 1, \Delta J = \pm 1$ (iv) $\Delta v = 0, \pm 1, \Delta J = 0, \pm 1$	CO1
Q 3	Fill in the blanks (a) The degeneracy for a rigid rotor ian an energy elevel with quantum number J is _____. (b) The zero point energy associated with rotation is _____.	CO1
Q 4	The wave number of the incident laser light in Raman spectroscopy experiment is 1440 cm^{-1}. If the wavenumber of Stokes line is 1410 cm^{-1}, what is the expected wavenumber of antiStokes line?	CO1

Q 5	Fill in blanks: Spectral lines are usually broad because various types of broadening such as (i)_____(ii)_____ (iii)_____	CO2
Q 6	Using cuvettes of 1 cm path length, a solution of 10^{-3} M solution of a dye solution shows 10% transmittance at certain wavelength. What is the molar extinction coefficient of the dye in $M^{-1}cm^{-1}$ at this wavelength?	CO2
SECTION – B **10 x 5 = 50 Marks** **1. Each question will carry 10 marks** **2. Instruction: Write short / brief notes/upload file**		
Q 7	Discuss the classical and quantum mechanical origin of Rayleigh, stokes and antistokes scattering line using diagram.	CO1
Q 8	Give the expression relating rotational constant to moment of inertia. If the rotational constant is 20 cm^{-1}, calculate the rotational energy of J=0, 1, 2.	CO1
Q 9	Explain the origin of splitting of lines of Na atomic spectra using spin orbit coupling. Use a diagram with proper labelling and term symbol to explain the spin orbit coupling of Na (Electronic configuration: $1s^2s^2sp^63s^1$).	CO2
Q10	(a)What are the selection rule for fundamental, first overtone, second overtone transitions? (b) The energy in cm^{-1} of the photon absorbed when a heteronuclear diatomic molecule goes from v = 0, J = 0 to v = 1, J =1. Assume the v = 0 and v =1 states have the same B values. Given that ω_e = 2000 cm^{-1}, B = 1.5 cm^{-1}, anharmonicity constant (χ_e) = 0.005.	CO2
Q 11	(a) Which of these molecules will show a pure rotational (microwave) spectrum: CCl_4, CH_3Cl, O_2, H_2O, C_6H_6, SF_6? Explain with proper reasoning. (b) Show the origin of P, Q, R branch in rotational-vibrational	CO2

	spectra?	
	Section – C **1 x 20 = 20 Marks** **1. Each Question carries 20 Marks.** **2. Instruction: Write long answers/ upload file.**	
Q 12	(a) The vibration of $^{1}H^{35}Cl$ molecule can be considered as simple harmonic oscillation. The force constant is 200 Nm^{-1}. Calculate the fundamental vibration frequency and the zero point vibrational energy of this molecule in joule. (Given: Plank constant = 6.626×10^{-34} Js). ***OR*** Draw all the vibrational normal modes of vibration of CO_2 molecule. Indicate the IR active vibrations of CO_2 molecule.	CO3 CO3
	(b) In rotational-vibrational spectroscopy for a polyatomic linear molecule (CO_2), what are parallel and perpendicular vibrations? Write the selection rule of rotational-vibrational spectra for parallel and perpendicular vibrations. ***OR*** Which of the following molecules has the lowest vibrational stretching frequency? Give justifications. (i) $^{1}H^{35}Cl$ (ii) $^{2}H^{35}Cl$ (iii) $^{1}H^{36}Cl$ (iv) $^{1}H^{39}Cl$	CO3 CO3