BMS COLLEGE FOR WOMEN AUTONOMOUS
BENGALURU-560004

END SEMESTER EXAMINATION – OCTOBER 2022
(CBCS)
M.Sc. in Chemistry- II Semester
Molecular Spectroscopy

Course Code: MCH204T **QP Code:21010**
Duration: 3 Hours **Max marks: 70**

Instruction: Answer Question No. 1 and any FIVE of the remaining.

1. Answer any ***TEN*** questions **(2×10 =20)**

a) Show that three reflection of ammonia constitute a class.

b) Prove that in BF_3 molecule $C_3\sigma_v \neq \sigma_v C_3$

c) Using the general matrix representation for $C_n(z)$. Write the matrix representations for C_3 and C_4 operation.

d) What do the Mulliken symbol B_{1g} and A_{2u} signify?

e) How many stretching and bending modes are present in CO_2 and SO_2 molecules?

f) Schematically sketch the bending modes of liner AB_2 molecule. What happens to this mode when AB_2 is bent?

g) How do you distinguish phosphorescence, fluorescence and Raman scattering from each other?

h) Define the term polarizability and depict the polarizability ellipsoid for H_2O molecule.

i) State the law of mutual exclusion.

j) Suggest a method for studying the vibration spectrum of N_2. Give reasons.

k) A molecule vibrates with a frequency of 1000 cm^{-1}. Express this energy in kJ/mole.

l) Explain the terms vibrational relaxation and internal conversion.

2. a). List the diagnostic symmetry elements and obtain the point group symmetry of the following molecules; i). H_2O, ii). CO_2, iii). C_2H_4, iV). C_6H_6, v). B_2H_6, vi). PCl_5

b). Write the matrix notations for the symmetry operations of C_{2h} point group. By matrix multiplication, prove that it is an Abelian group. **(6+4)**

3. a). Construct the character table for the operations of C_{3v} point group. Explain each area in detail.

b). Using perturbation theory, obtain the selection rules governing the vibrational transitions of an anharmonic oscillator. **(5+5)**

4. a). Explain the terms: Overtones, Combination bands and Fermi resonance.

b). Outline concept of normal modes of vibration of a molecule. Sketch schematically the normal modes of AB_3-planar molecule and comment on its IR and Raman activity. **(4+6)**

5. a). Write briefly on the main components of infrared spectrometer.

b). Describe the classical theory of Raman Effect.

c). A strong infrared absorption band is observed at 2991 cm^{-1} for $^{1}H^{35}Cl$ molecule. Calculate the force constant for this molecule. **(4+3+3)**

6. a).The spacing between the successive line in the microwaves spectrum of CO is 3.84235 cm^{-1}.Obtain the bond length of CO. ($h=6.626 \times 10^{-34}$ Js; c= 3 x 1010 m/s; $m_H=1.67X10^{-27}$ kgs)

b). Write the expression for the rotational energy of;

i). a rigid symmetric top and

ii). The non-rigid symmetric top.

Make schematic plots of the microwave spectra of the two by giving the selection rules. **(5+5)**

7. a). State and explain the selection rules for the electronic transition.

b). Explain the origin of O and S branches in the vibrational-rotation Raman spectrum of a diatomic molecule. **(4+6)**

8. a). Give comprehensive notes on: Fronck-Condon principle and Fortrat diagram.

b). Depict the electronic configuration of the ground and excited states of HCHO molecule. Explain the electronic transitions involved in it. **(5+5)**

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