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AR-19

M.SC

M.Sc 1<sup>ST</sup> SEMESTER REGULAR EXAMINATIONS, NOV/DEC 2019-20

CHPC104-SPECTROSCOPY-I

Time: 3 Hours

Max Marks: 80

The figures in the right hand margin indicate marks.

SECTION A

- Q.1 Answer any four of the following: [ 4 X4 =16]
- a Write the expression of energy of an electron in hydrogen atom? Using this equation calculate the energy of 4s and 3d orbital.
  - b What is mutual exclusion principle? Taking example of CO<sub>2</sub> molecule, explain which vibrational states are active in IR and which are active in Raman.
  - c What is zero field splitting in EPR? Explain with an example.
  - d How the atom substitution can be detected using rotational spectra? Explain with an example what happens to the rotational spectra, when Hydrogen is substituted with Deuterium.
  - e What is Kramer's degeneracy? Explain with an example.
  - f A free Mössbauer nucleus of mass 100.6 amu emits radiation of wavelength 0.1 nm. Calculate the recoil velocity and Doppler shift.

OR

2. Answer all questions from the following [2 x 8 =16]
- a With the help of morse potential energy curve for a diatomic molecule and label zero point and dissociation energy.
  - b Which solvent between CCl<sub>4</sub> and CH<sub>3</sub>CN, will you choose to study vibrational fine structures? Explain with reason.
  - c When F<sub>2</sub> molecule is exposed to Hg lines of wavelength 404.7 nm and 435.8 nm, the stokes line appears at 419.9 and 453.4 nm. Calculate the ground state vibrational frequency of F<sub>2</sub>.
  - d The half-life of <sup>67</sup>Zn nucleus is 9400 ns. Calculate the line-width in  $\gamma$ -ray emission.
  - e Define polarizability. What is its importance in IR spectroscopy?
  - f How can you detect the change of acid to amide using IR spectroscopy?
  - g What is photoelectric effect? Explain with suitable diagram.
  - h Name any two factors that affect g value in EPR spectroscopy.

SECTION-B

3. Answer all Questions: [16 x4 =64]
- a Discuss how atomic and molecular spectra are different. Discuss the spectra of hydrogen atom.

OR

- b What is Frank Condon Principle? With suitable diagrams explain the intensity of vibrational-Electronic spectra.
- 4.
- a Discuss the conditions of a diatomic molecule to be active in IR spectra. Taking help of energy levels equation(s) and selection rules, draw and discuss an energy level diagram for the rotational - vibrational spectrum of a diatomic molecule.

OR

- b How can you explain the origin of Raman lines in the view of classical and quantum theory? With suitable example, explain, how rule of mutual exclusion principle helps in providing information regarding structure of a molecule.



- 5.
- a What is Born-Oppenheimer approximation? Considering a diatomic molecule to be a rigid rotator, calculate the expression for interatomic distance in a diatomic molecule. Calculate the bond distance for HCl if the rotational lines are equally separated by  $20.70 \text{ cm}^{-1}$  (given: atomic weight of Cl is 35.5 amu)

OR

- b Discuss the principle of photoelectron spectroscopy. Draw and discuss the PES of  $\text{N}_2$  molecule in the light of the principles.

6.

- a Describe the basic principle of ESR spectroscopy. Discuss the factors those affect intensity, line width, position and splitting of a spectra.

OR

- b What is basic principle of Mössbauer spectroscopy?  
Consider the following case and answer the following questions. A particular Mossbauer nucleus has spin  $5/2$  and  $3/2$  in its excited state and ground state respectively. Explain with proper diagrams, into how many lines will the gamma ray spectrum split if : i) The nucleus is under the influence of internal electric field gradient but no magnetic field is applied; ii) There is no electric field gradient at the nucleus but an external magnetic field is applied; iii) Both an internal field gradient and an external field gradient is present.