Reg. No. | | | | | | | | | |

CH/AC/OC/CA S 406

I Semester M.Sc. Examination, December 2018
CHEMISTRY/APPLIED CHEMISTRY/ORGANIC CHEMISTRY/ ANALYTICAL CHEMISTRY
(CBCS : 2016 – 17 Syllabus)
Molecular Spectroscopy and Diffraction Techniques

Time : 3 Hours Max. Marks : 70

Note : *i) Answer Part – **A** and **any four** questions from Part – **B**.*
*ii) Figures to the **right** indicate marks.*

PART – A

Answer **all** the following sub-divisions. **(9×2=18)**

1. a) Account for the fact – 'Transition probability and population of states are major factors in deciding the intensity of spectral lines'.

   b) Justify the fact that "Microwave spectroscopy can readily distinguish the presence of isotopes in a sample even though it cannot detect the presence of particular grouping".

   c) Comment on the importance of force constant in determining the bond length.

   d) Write the selection rules to be adopted to get parallel and perpendicular modes of vibrations in the IR spectrum of a molecule.

   e) With an illustrative example show that the centre of symmetry has an effect on the intensity of alternate lines in the P and R branches.

   f) The fundamental vibrational frequency of HCl is 2890 cm^{-1}. Calculate the force constant of this molecule. (The atomic masses : $^{1}H = 1.673 \times 10^{-27}$ Kg, $^{35}Cl = 58.06 \times 10^{-27}$ Kg).

   g) What is Ewald sphere ? Give its physical significance.

P.T.O.

h) Explain the working principles of transmission electron microscope.

i) How do you estimate the wavelength of an electron beam ?

PART – B

Answer **any four** questions. **(4×13=52)**

2. a) Explain the effect of isotopic substitution on the energy levels and rotational spectrum of a rigid diatomic molecule.

b) Differentiate between harmonic and anharmonic osicllators with the help of potential energy curves.

c) The pure rotational spectrum of gaseous HCl consists of a series of equally spaced lines by 20.80 cm^{-1}. Calculate the internuclear distance of the molecule (h = 6.626 $\times 10^{-34}$ Js, ^{1}H = 1.673 $\times 10^{-27}$ Kg, ^{35}Cl = 58.06 $\times 10^{-27}$ Kg, C = 3×10^{8} ms^{-1}, I = 10.40×10^{2}). **(4+4+5)**

3. a) The spectrum of HCl shows very strong absorption at 2886 cm^{-1}, a weaker one at 5656 cm^{-1} and a very weak one at 8347cm^{-1}. Find equilibrium frequency, anharmonicity constant and force constant.

b) Explain the microwave spectrum of a rigid diatomic rotator.

c) Draw and explain the rotational vibrational energy levels for any symmetric top molecule using the principle of Born-Oppenheimer approximation.

(3+5+5)

4. a) Explain the Raman effect based on quantum theory of radiation.

b) What do you mean by 'mutual exclusion principle' ? Explain how is it useful in the structural elucidation of a molecule.

c) The spacing between lines in rotation Raman spectrum of a diatomic molecule in 12 cm^{-1}. What is the Raman shift of first Stokes line ? **(4+6+3)**

5. a) Explain the Raman activity of vibrations of H_2O and N_2O.

   b) Explain the rotational Raman spectrum of a symmetric top molecule.

   c) With a neat sketch explain the working of Raman spectrometer. **(5+5+3)**

6. a) Describe the Laue method of study of X-ray diffraction of single crystals.

   b) Draw and explain the intensity Vs. sin (θ/λ) plots concerned with X-ray diffraction of atoms and molecules.

   c) Write a note on the applications of neutron diffraction. **(4+5+4)**

7. a) Explain any four important factors which control the diffracted X-ray beam intensity.

   b) Discuss the theory and applications of electron diffraction.

   c) Give an account of the systematic absence. **(4+5+4)**
