



I Semester M.Sc. in Chemistry Degree Examination, September 2016
CHEMICAL SPECTROSCOPY

Time : 3 Hours

Max. Marks : 80

Instruction : Answer **any eight** questions from Part – I and **any four** full questions from Part – II.

PART – I

(2×8=16)

- i. Write two differences between harmonic and anharmonic oscillators.
- ii. Explain the differences between energy levels in free atom and molecules.
- iii. When and why the rotational motion of a diatomic molecule is considered to resemble that of rigid and non-rigid rotators ?
- iv. What are auxochrome ? Give two examples.
- v. What is meant by bathochromic shift ?
- vi. What is zero point energy ?
- vii. What are overtone bands in vibrational-rotational spectroscopy ?
- viii. What is chemical shift in NMR spectroscopy ?
- ix. Outline the differences between NMR and NQR.
- x. Which of the following atoms does not exhibit NMR spectroscopy ?
 ^{12}C , ^{15}N , ^{13}C . Explain why ?

PART – II

1.
 - a) Explain the consequences of interaction of molecule with different regions of electromagnetic radiation.
 - b) Explain the basic principle of ESR spectroscopy.
 - c) Describe three wave nature properties of electron. **(4+6+6=16)**
2.
 - d) How do you distinguish between symmetric top and asymmetric top molecules ?
 - e) Predict the effect of isotopic substitution on rotation spectra and the information that can be obtained from such a study.
 - f) Write a note on Franck-Condon principle. **(4+6+6=16)**

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3. g) Derive the equation for vibrational energy of simple harmonic oscillator.
h) Derive the expression for the calculation of frequency for the vibrational-rotational spectra of diatomic molecule.
i) For $^1\text{H}^{35}\text{Cl}$; Bond length is 127.5 cm, force constant is 516.3 N/m and atomic masses of $^1\text{H} = 1.673 \times 10^{-27}$ kg, $^{35}\text{Cl} = 58.066 \times 10^{-27}$ kg. Calculate the zero-point energy and rotational constant B. **(4+6+6=16)**
4. j) Explain shielding and deshielding effect in NMR.
k) Write a note on spin lattice and spin-spin relaxation process.
l) Explain principle of NQR. **(4+6+6=16)**
5. m) Explain the significance of Hyperfine interaction in ESR spectroscopy.
n) Discuss the factors that determine the intensities of rotational lines for linear molecules.
o) Discuss in detail about symmetry restrictions in electronic transition. **(4+6+6=16)**
6. p) Explain why PhMe, Ph₂CH₂ and Ph₃CH have similar UV spectra ($\lambda_{\text{max}} \sim 262$ nm).
q) What is coupling constant ? How do you distinguish cis and trans isomers with the help of NMR spectroscopy ?
r) Write a note on the number of modes of possible vibrations of poly atomic molecules.
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