



BM-2030-31 Seat No. \_\_\_\_\_

**M. Sc. (Sem. II) Examination**

**April / May - 2014**

**CHN-504 (A) & (B) : Chemistry : Paper - XI**

**1. 504 (A) : Spectroscopy**

**2. 504 (B) : Computers For Chemists**

Time : 2 Hours]

[Total Marks : 50

**1. 504 (A) : Spectroscopy**

1 Answer any five 20

- (a) By giving suitable examples, explain overtones, hot bands and combination bands.
- (b) Give an account on Rotational Raman spectra.
- (c) Explain 'P' branch and 'R' branch.
- (d) Give the principle and applications of Raman spectroscopy.
- (e) Explain why OCS molecule is microwave active but  $\text{CO}_2$  is not. Explain whether  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$  (isotope substitution) will be active or inactive in microwave spectroscopy by giving the reason.
- (f) Give an account on normal modes of vibration.
- (g) Give chemical analysis by microwave spectroscopy.
- (h) Give an account on force constant and bond strength using vibrational spectroscopy.

2 Answer any five

20

- (a) Explain spin-spin interaction and inter molecular exchange by taking the example of PMR of ethanol molecule in different conditions.
- (b) Give the instrumental details of NMR spectroscopy.
- (c) Illustrate and elaborate the concept of chemical shift.
- (d) Give an account on the importance of coupling constant
- (e) Illustrate the applications of  $^{13}\text{C}$  NMR (CMR).
- (f) Give an account on  $^{19}\text{F}$  NMR with applications.
- (g) Discuss the use of NMR in medical diagnostics.
- (h) Write a note on Larmor precession.

3 Answer any five (in 3 to 5 lines)

10

- (a) What is Fermi Resonance?
- (b) Explain and draw  $^1\text{H}$ -NMR spectrum of  $\text{Br-CH}_2\text{-CH}_2\text{-CH}_2\text{-CN}$ .
- (c) What is the importance of depolarization ratio?
- (d) Explain the meaning of Fourier Transform.
- (e) What are meanings of elastic and inelastic scatterings?
- (f) What is spin-spin relaxation?
- (g) Explain breakdown of Born-Oppenheimer approximation.
- (h) What is Bohr magneton?
- (i) What is Stark effect?
- (j) What are nuclear spin and isotopic abundances of  $^{13}\text{C}$  and  $^{31}\text{P}$ ?
- (k) What is Morse potential energy diagram?

## 2. 504 (B) : Computers For Chemists

1 Write any four :

- (1) What is memory? Explain types of memories in brief.
- (2) What is importance of algorithm in programming language. Explain it with any example.
- (3) Explain IF & GOTO statement with example.
- (4) What is operator? Explain all operators with example.
- (5) Describe the difference between function & Procedure.

2 Write any four :

- (1) Explain linear simultaneous equations to solve secular equation within Huckel theory.
- (2) Write down solution for Van des Waals equation.
- (3) What is matlab? Explain any one application of matlab.
- (4) Explain Monte Carlo method.
- (5) Write down the features of FOXPRO.

- 3 Write any five :
- (1) RAM.
  - (2) Any 3 name of I/o devices.
  - (3) Constant
  - (4) Use of Header/Footer in MS word
  - (5) Flow-chart
  - (6) Difference between windows and UNIX O.S.