Code No. : **9273/AB**

FACULTY OF SCIENCE

M.Sc. II Semester Examination, May/June 2012

CHEMISTRY

Paper – IV : Computers in Chemistry and Spectroscopy

Time : 3 Hours] [Max. Marks : 80

Note : *This question paper consists of **two** parts. Part **A** is Computers in Chemistry. Part **B** is Spectroscopy. Write Part **A** and Part **B** in **separate** answer books. Answer **all** questions.*

PART – A

(Computers in Chemistry)

SECTION – A **(1×8=8 Marks)**

1. a) Write a brief note on input and output devices.

   b) What are the steps involved in testing a source program in C ?

SECTION – B **(1×12=12 Marks)**

2. a) Give the syntax for printf( ), scanf ( ) and puts with examples.

   b) Write the listings of a C program for roots of a quadratic equation.

   OR

   c) Define an array. Write the syntax for a two dimensional array.

   d) Write the listings of a C program for first order rate constant from kinetic data.

PART – B

(Spectroscopy)

SECTION – A **(3×8=24 Marks)**

1. a) Write a note on lanthanide shift reagents.

   b) How nmr spectrum can be simplified by deuterium exchange ?

2. a) Explain nitrogen rule with examples.

   b) What are meta stable peaks ? How can they be identified ?

3. a) What are the characteristic fragmentation pattern of cyclo alkanols ?

   b) What is ortho effect ?

SECTION – B **(3×12=36 Marks)**

4. a) Explain how nmr spectra can be simplified by
      i) increasing the field strength and
      ii) double resonance.

   b) What is NOE ? Give examples.

OR

   c) Sketch the ^{1}H and ^{13}C nmr of $^{13}CH_4$. Explain its splitting pattern.

   d) What are the applications of ^{19}F nmr spectra ?

5. a) Describe the working of electron spray ionisation mass spectrometer.

   b) What is the principle involved in LC - MS interface ? What are its advantages and disadvantages ?

OR

   c) Explain the principle involved in quadrupole mass analyzer.

   d) What is FAB technique ? What type of molecules can be analyzed by this technique ?

6. a) An organic compound ($C_8H_8O_2$) gave peaks at m/z 136, 105, 77 and 51. Identify the compound and indicate the fragmentation pattern.

   b) Explain the fragmentation pattern of aliphatic amines with suitable example.

OR

   c) Explain McLafferty and double McLafferty rearrangements with suitable examples.

   d) Explain the mass spectral fragmentation of $ReBr(CO)_5$.