



Code No. : **631/AB**

FACULTY OF SCIENCE
M.Sc. II Semester Examination, April/May 2013
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) Discuss about different operators used in C language.
b) Explain the different types of output devices.

SECTION – B

(1×12=12 Marks)

2. a) Explain for loop with its syntax and write the suitable C program by using for loop.
b) Write a program to calculate first-order rate constant from kinetic data.

OR

- c) Discuss the syntax for printf(), scanf() and gets() with examples.
d) Write a C program for roots of quadratic equation.

PART – B

(Spectroscopy)

SECTION – A

(3×8=24 Marks)

1. a) Write the applications of solid state NMR.
b) Discuss about deuterium exchange and double resonance technique.

(This paper contains 2 pages)



2. a) Explain the principle involved in the electron spray ionization (ESI) mass spectrometry.
b) Discuss the applications of the GC-MS.
3. a) Explain the mass spectral fragmentation of ReBr_2 .
b) Write the mass spectral fragmentation of benzoic acid.

SECTION – B

(3×12=36 Marks)

4. a) Explain the use of Lanthanide shift reagents in simplification of NMR spectra.
b) Explain the applications of ^{32}P NMR spectra.

OR

- c) Explain the coupling interactions of ^{19}F with other spin active nuclei.
 - d) Discuss about first and non first order spectra.
5. a) Write is the principle involved in MALDI ? Mention its applications.
b) Discuss the following with suitable examples :
 - i) isotopic labelling
 - ii) molecular ion peak

OR

- c) Discuss about general modes of fragmentations.
 - d) What is FAB technique ? What type of molecules analyzed by this technique ?
6. a) Discuss McLafferty rearrangement with suitable examples.
b) Explain retro Diels-Alder fragmentation with examples.

OR

- c) Discuss the Ortho effect.
- d) Mass spectrum of $\text{C}_4\text{H}_8\text{O}$ shows the following peaks m/z 72(M^+), 71, 44, 43, 29. Write the fragmentation pattern and deduce its structure.