Code No. 9223

FACULTY OF SCIENCE

M.Sc. II - Semester Examination, April / May 2014

Subject : 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 x 8 = 8 Marks)

1 a) Explain the different types of input devices.

b) Write a note on If and If - else statements.

Section – B (1 x 12 = 12 Marks)

2 a) Explain about Constants and Variables used in C language.

b) Write a program to calculate dissociation constant of acetic acid from conductance data.

OR

c) Discuss While loop with its syntax and write the suitable C program by using While loop.

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

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PART – B
(Spectroscopy)

Section – A (3 x 8 = 24 Marks)

1 a) Write a note on Nuclear Overhauser Enhancement (NOE).
b) How NMR spectrum can be simplified by using Lanthanide shift reagents?

2 a) How do you determine molecular formula of a compound from its mass spectra.
b) Discuss Nitrogen rule with examples.

3 a) Write the mass spectral fragmentations of benzaldehyde.
b) Discuss the mass spectral fragmentation of $ReBr(CO)_5$.

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Section – B (3 x 12 = 36 Marks)

4 a) Discuss the applications of ^{19}F NMR spectra.
b) Explain the first order and non first order spectra with examples.

OR

c) Explain the use of chiral NMR solvents.
d) Discuss about Magic Angle Spinning (MAS) and its applications.

5 a) Write a note on meta stable ion peaks.
b) What is the principle involved in GC-MS? Write its applications.

OR

c) Explain the working of electron spray ionization mass spectrometer.
d) What is FAB technique? What type of molecules are analysed by this technique?

6 a) Discuss the fragmentation patterns of aliphatic alcohols with suitable examples.
b) Explain retro Diels-Alder fragmentation with examples.

OR

c) Explain McLafferty rearrangement with suitable examples.
d) The mass spectrum of o –nitrotoluene shows a substantial peak at m/z 120, similar analysis of α, α, α-trideutero-o-nitrotoulene does not give a peak at m/z 120 but rather at m/z 122. Explain.

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