#### PD - 265 CV-19

## (532) M.Sc. CHEMISTRY (SECOND SEMESTER)

# **Examination JUNE 2021**

## Compulsory/ Optional

### Group-

### Paper- IV

Name/Title of Paper- SPECTROSCOPY & COMPUTER FOR CHEMISTS

Time: Three hours

Maximum Marks-80 Minimum Passing Marks-29

Note: Answer From Both the Section as Directed. The Figures in the right-hand margin indicate marks.

#### Section-A

1. Answer the following questions:

1x10=10

- a) Which electronic state is to be expected of lowest energy in d<sup>2</sup> case?
- b) Write the mathematical formula for the calculation of number of microstates?
- c) Write the name of element which mostly gives photoelectric effect?
- d) Identify different types of hydrogen in toluene with reference to NMR spectroscopy?
- e) Who invented photo acoustic spectroscopy?
- f) How the lattice spacing (d) is connected to cell edge (a) for simple cubic lattice?
- g) Processing is done in which part of computer?
- h) How many digits is present in Binary systems?
- i) What is the name of first menu of MS-Excel?
- j) Who is the father of 'C' Language?

2. Answer the following questions:

2x5=10

- a) In a hydrogen atom, an electron jumps from a third orbit to the first orbit. Find out the frequency of the spectral fine?
- b) Write four complications in NMR analysis?
- c) The intercept ratios of a crystal plane are a:b:∞c. Calculate the Miller indices of the plane?
- d) Write short notes on Algorithm & Flow chart?
- e) Explain how you can prepare a graph and chart by using MS-Excel?

#### Section-B

Answer all questions:-

12x5=60

3. Describe scheme of vector coupling of orbital angular momentum and spin angular momentum and hence total angular momentum for p<sup>n</sup> d<sup>n</sup> configuration?

Or

Discuss the basic principles, classifications and instrumentation of photo electronic spectroscopy?

- 4. (a) Explain the factors affecting the chemical shift in NMR spectroscopy?
  - (b) Discuss the instrumentation for photo acoustic spectroscopy?

Or

(a) Which of the following system will show Electron spin Resonance spectroscopy and why:-

 $O_2$ ,  $O_2^+$ ,  $O_2^-$ , NO, CH<sub>3</sub> radical and  $C_{O_2}$ 

- (b) Explain the instrumentation and applications of Nuclear Quadruple Resonance spectroscopy?
- 5. (a) Derive Bragg's equation?
  - (b) The interplanar spacing of a crystal was found to be 1.85  $A^0$ . If the first order reflection takes place at an angle of  $30^0$  find out the wavelength of X-rays? [Given Sin  $30^0 = 0.5$ ]

Or

- (a) Explain Ramchandran diagram of protein?
- (b) Discuss Laue's method of X-ray structural analysis of crystal?
- 6. (a) Explain constants and variable used in "c" programming?
  - (b) Write short notes on "pointers"?

Or

What are operating systems? Discuss in detail the salient features of any one of the operating systems that are prescribed in your syllabus?

- 7. Write a program in "c" to execute results for calculation of:-
  - (a) pH Titration
  - (b) Secular equation

Or

Describe the facilities available in word processor? Write the salient features and uses of M.S.-Word?