



**LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034**

**M.Sc. DEGREE EXAMINATION – CHEMISTRY**

THIRD SEMESTER – APRIL 2018

**CA 3900- COMPUTERS IN CHEMISTRY**

Date: 05-05-2018  
Time: 09:00-12:00

Dept. No.

Max. : 100 Marks

**PART-A**

**Answer ALL Questions**

**10\*2=20**

- 1) What are keywords? Give any 4 keywords.
- 2) List the data types used in C language.
- 3) What is Debroglie wavelength?
- 4) State Huckel Mo theory.
- 5) Convert the following into C expression  
$$X1 - X2 = 0.18(E1 - (E2 * E3)^{1/2})^{1/2}$$
- 6) Write a structure for Born-Lande equation.
- 7) Write a control statement to determine the method using Woodward Hoffman rule for electrolytic reactions.
- 8) Write a for loop to calculate empirical formula.
- 9) What is the use of Biuret method?
- 10) Write any four applications of computers in chemistry.

**PART-B**

- 11.a) Explain the different operators used in 'C'. Give examples.  
(or)  
b) Illustrate SWITCH CASE with an example.
- 12.a) Write a C program using arrays to find the heat of reactions.  
(or)  
b) Write a C program to calculate interplanar spacing of a crystal using Bragg's Law.
- 13.a) Write a C program to determination of Lattice energy of sodium chloride using BORN-LANDE equation.  
(or)  
b) Write a C program to calculate the half and average life.
- 14.a) Write a C program to determine the wave length maximum.  
(or)  
b) Write a C program to estimate the percentage of C,H,O in organic compound using structures.

15.a) Write a C program to calculate the hydrogen ion concentration using arrays.

(or)

b) Write a C program to determine calcium using titrimetric method.

### **PART-C**

**Answer any TWO Questions**

**2\*20=40**

16. Explain the categories of functions with example

17.a) Write a C program to find the secular equation for ethylene using arrays.

b) Write a C program to find the solubility of sparingly soluble salt.

18.a) Write a C program to calculate the molecular weight using arrays.

b) Write a C program to :-

i. estimate the Glucose level using orthotoludine method.

ii. estimate percentage of protein.