

LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION - CHEMISTRY

THIRD SEMESTER – NOVEMBER 2007

CS 3902 - COMPUTERS IN CHEMISTRY

AK2

Date : 06/11/2007
Time : 9:00 - 12:00

Dept. No.

Max. : 100 Marks

PART – A

Answer ALL of the following:

10 x 2 = 20

(Note: program should not be written for part – A)

1. Define keyword. Give any eight key words.
2. Define array. How will you declare an array?
3. Differentiate while and do-while statement.
4. Convert into C expression
$$P(x) = F_0 + 2 \sum F_h \cos(2\pi hx).$$
5. Convert into C expression
 - a. $X1 - X2 = 0.18(E1 - (E2 * E3)^{1/2})^{1/2}$
6. Write a structure for Born-Lande equation.
7. Write a if statement to determine the method using Woodward – Hoffman rule for electrolytic reactions.
8. Write a switch case to estimate either N or O or S.
9. Write any four application of computer in chemistry.
10. Name any four header files used in C.

PART – B

Answer ALL of the following:

5 x 8 = 40

11.a. Explain the switch statement with an example.

(OR)

b. Explain the Break and Continue statements with example.

12.a. A crystal lattice has an interplanar distance of 0.235 nm. Write a C program to calculate the wavelength of the x-ray when it falls at an angle of 19.0 degree for a first order reflection.

(OR)

b. Write a C program to calculate the heat of reactions at constant volume and constant pressure relationship.

[PTO]

13.a. Write a C program to calculate the Lattice energy of crystal using Bornlande equation.

(OR)

b. Write a C program to determine

- i. the concentration of a solution using Beer Lambert law
- ii. Binding energy

14.a. Write a C program to determine the empherical formula.

(OR)

b. Apply Wood ward Hoff mann rule in pericyclic reaction to determine the method and mode of rotation. Write a C program for the above rule.

15.a. Write a C program to calculate the amount of calcium in a given substance using Titrimetric method.

(OR)

b. Write a C program to determine the PH level

PART – C

Answer any TWO of the following:

2 X 20 = 40

16. Explain the control statements with example for each.

17.a. Write a C program to find the density of electron.

b. Write a C program to calculate the electronegativity of atoms using bond energy data for N sets.

18.a. Write a C program to estimate the percentage of N, S, O in organic compound.

b. Write a C program to determine proteine using Biuret method.
