6. (a) Discuss the application of computers in chemistry. Write a programme to calculate the radioactive decay constant.

OR

(b) Discuss the various elements in computer language. Write a programme to calculate van der Waals equation.

2016
(January)

Time : 3 hours

Full Marks : 80

The figures in the right-hand margin indicate marks.

Answer from both the Sections as per direction.

(BASIC PHYSICAL CHEMISTRY – I)

Section – A

1. Answer any **four** of the following : 4×4 = 16

(a) Show that sum of square of characters in any irreducible representation is equal to h.

(b) Write the postulates of Quantum Mechanics.

(c) Why certain combinations of atomic orbitals are not allowed ? What are they ?

(d) Show that for a particle moving in a one dimensional box of length a, average value of x, $\langle x \rangle = a/2$.

(e) Show that $[\hat{L}^2, \hat{L}_z] = 0$.

(f) Discuss the variables and constants in C programming.

OR

2. Answer **all** questions : 2×8 = 16

(a) State great orthogonality theorem.

(b) Why S orbitals are spherical in shape ?

(c) List the symmetry elements for the molecules (i) B_2H_6 and (ii) C_2H_2.

(d) What do you understand by LCO principle ?

(e) What is the difference between Ψ and $4\pi^2r^2\Psi^2$?

(f) What are logical variables ?

(g) What is conditional statement in C language ?

(h) What do you mean by direct product ?

Section – B

Answer **all** questions : 16×4 = 64

3. (a) Deduce the character table for C_{3v} point group. Based on the characteristics of irreducible representation, set up the

irreducible presentation of the point group C_{3v}.

OR

(b) What information is conveyed by character table ? Explain by taking suitable example. List all the rules for writing Mulliken's symbol of irreducible representation.

4. (a) Construct a molecular orbital energy level diagram for the $[PtCl_4]^{-2}$ species.

OR

(b) Classify the metal and ligand orbitals $ML_5(D_{3h})$ complex into their appropriate σ symmetries.

5. (a) State variation theorem. Calculate the energy of Helium atom using linear variation principle.

OR

(b) Set up specular determinant for butadiene. Find out electron density, charge density, bond order of butadiene.