7. Explain how to visualize the wave functions obtained from the Schrödinger equation solution. What adjustments or enhancements can be made for clarity and presentation using Python ? 15

8. Explain how machine learning can be applied in the field of chemistry. Provide examples of its applications in material science or drug design. 15

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[This question paper contains 4 printed pages]

Your Roll No. : .....

Sl. No. of Q. Paper : **5701** **I**

Unique Paper Code : 2173012015

Name of the Paper : DSE : Application of Computers in Chemistry

Name of the Course : **B.Sc.(Hons.) Chemistry**

Semester : IV

Time : 3 Hours ***Maximum Marks : 90***

Instructions for Candidates :

(a) Write your Roll No. on the top immediately on receipt of this question paper.

(b) **All** questions carry equal marks. There are eight questions in all. Attempt any **six** questions.

(c) Each question carries **15** marks.

5×3=15

1. (i) What are the main components of a computer ?

(ii) What is the difference between hardware and software ?

(iii) What is a hard drive and how does it differ from an SSD ?

(iv) What is the role of a firewall ?

(v) What are the main types of computer networks ?

3×5=15

2. (a) What are the software used in Chemical Sciences, Explain.

(b) Write the languages used in computer for programming. Explain.

(c) Write the number systems used in computer. Explain.

3×5=15

3. (a) Describe the role of Python as a tool in Chemistry.

(b) Explain Python as a programming language in computer.

(c) How Python is a better programming language for artificial intelligence and machine learning. 3×5=15

4. (a) How Matplotlib can be used to create a histogram. What are the key parameters available in the plt.hist() function ?

(b) How to customize plots in Matplotlib ? Discuss different customization options such as colors, line styles, markers and adding annotations available in Matplotlib.

(c) What are subplots and how can they be used to create multi-plot figures in Matplotlib ? Explain with an example.

3×5=15

5. (a) Differentiate lists and tuples in Python with examples of illustrate their usage.

(b) What do you understand by Object-Oriented Programming (OOP) in Python ? Explain with example.

(c) Explain how memory is managed by Python and illustrate memory management concepts such as reference counting and garbage collection with an example.

6. How can you solve the time-independent Schrödinger equation for a one-dimensional potential well using Python ? Provide an example using the finite difference method. 15