

[This question paper contains 12 printed pages]

Your Roll No. :

Sl. No. of Q. Paper : **1186** **I**

Unique Paper Code : 2173010006

Name of the Paper : Application of Computers
in Chemistry

Name of the Course : **B.Sc.(H.)**

Semester : V

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) Question No.1 is compulsory. Do any **five** questions from the rest of the questions. Answer **six** questions in **all**.
- (c) **All** questions carry equal marks.

1. (a) Explain with examples, what each of the below functions do : 5

- (i) chr ()
- (ii) ord ()
- (iii) round (m, n)
- (iv) min ()
- (v) max ()

P.T.O.

(b) What would be the output of the below lines of code :

2×5=10

(i) `print ("chemistry" * 2 + ".join(['p', 'y', 't', 'h', 'o', 'n']))`

(ii) `if (abs (-2) >= 2 and ( 5 % 3 == 2)) :`
`print ('Yes')`

`else :`

`print ('No')`

(iii) `for x in range (2) :`

`y = 0`

`while y < 2 :`

`print (x * y)`

`y = y + 1`

(iv) `import numpy as np`

`list1 = ["He", "Li", "B"]`

`list2 = ["F", "Cl", "Br"]`

`nparray = np. array ([list1, list 2])`

`print (nparray. shape)`

(v) `import matplotlib. pyplot as plt`

`import numpy as np`

`x = np. linspace (-10, 10, 1000)`

`y = 2 * x + 50`

`plt. plot (x, y)`

2. (a) Write the full form of below acronyms :

1×5=5

(i) NUMPY

(ii) HDD

(iii) AI

(iv) DOS

(v) ALU

(b) Write the below algebraic/scientific expressions in Python friendly format :

1×=5

(i)
$$\frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

(ii)
$$4\pi \left(\frac{M}{2\pi RT} \right)^{3/2} v^2 e^{\left\{ \frac{Mv^2}{2RT} \right\}}$$

(iii) $(2 + 3i)$

(iv) $RT \ln K$

(v) $\log_{10}[A] - kt$

(c) Six parts of the below program are missing and shown as underlines. Find all the six missing part : 5

```
def throw_dice () :  
# Simulate throwing two dice by randomly
```

```

selecting a number from 1 to 6
player1 _throw = _____
player 2 _ throw = _____
print ("Player 1 throws : ",player1_throw)
print ("Player 2 throws : ",player2_throw)
# Determine the winner based on who gets
the larger number

_____
print ("Player 1 wins !")

_____
print ("Player 2 wins !")

_____
print ("It's a tie !")
# Run the dice – throwing game
throw _dice ( )

```

3. (a) What is the difference between : $1 \times 5 = 5$
- (i) Storage and Memory
 - (ii) Interpreted Language and Compiled Language
 - (iii) plt. bar and plt. barh ()
 - (iv) str. find () and str. rfind ()
 - (v) numpy. arange () and numpy. linspace ()

(b) Write python programs to :

(i) plot a simple sine curve from -2 radians
to + 2 radians 2.5

(ii) convert any given angle from degrees
to radians using function 2.5

(c) Write a Python program to evaluate the

integral $\int_5^{10} (x^2 - 3x + 2) dx$ using the

Trapezoidal method of numerical
integration. There is no need to show the
output. 5

4. (a) Which of the following is a valid Python
variable name. Wherever you mention it is
invalid, please provide a one - line reason
why it is invalid. 1×5=5

(i) include

(ii) theta % 2

(iii) 2 sigma

(iv) Print

(v) i_am_a_really_really_long_python_variable_name

- (b) Write a Python program to identify **Armstrong numbers** using string manipulations. An **Armstrong number** is a number that is equal to the sum of its own digits each raised to the power of the number of digits in the number. 5

OR

Given the periodic table of elements in the dictionary format as follows :

$P = \{1 : \text{"H"}, 2 : \text{"He"}, 3 : \text{"Li"}, \dots, 11.8 : \text{"Og"}\}$

Write a Python program to find the first 8 **Prime Numbers** and then print the symbols of elements corresponding to these numbers from the above periodic table P as a list. For example, the list's first two elements would be ["He", "Li"....] 5

- (c) The below program produces FIVE lines of output. Provide all 5 lines of output in the **correct** sequence : 5

$a = (2, 3)$

$b = \{3, 4, 5\}$

$c = [2, 3, 4, 5]$

$d = \{2 : \text{"He"}, 10 : \text{"Ne"}, 18 : \text{"Ar"}\}$

```

print (c. pop ( : ))
print (c)
b. add (4)
b. add (6)
print (b)
a = a * len (b)
print (a)
print (len (d.keys ( ) ))

```

5. (a). Find and correct the errors in the below lines

of code : 1×5=5

- (i) s = python
- (ii) x = y + z;
- (iii) print "quantum"
- (iv) for i = 1 to 4 print i
- (v) import numpy into up

(b) Do any **two** parts from the below 3 parts for this question ; 2,5×2=5

Write python programs (without the use of numpy/scipy/statistics) to

- (i) Find the average and standard deviation of a given list of numbers
 - (ii) To Print the first 10 terms of a Fibonacci series
 - (iii) Print the difference between the first 10 odd numbers and the first 10 even numbers and show that it will be zero. Please exclude 0 from your computation.
- (c) Write a Python program to solve the equation $x^3 + x^2 + 2 = 0$ using **Newton-Raphson method** with the guess value as -2. 5

6. (a) Write the output of the below lines of code :

1×5=5

- (i) `print (["chemistry", "physics", "maths" ] [:1])`
- (ii) `print ([4, 5, 6, 7] [1 :2])`
- (iii) `print ("quantum chemistry" [:: -1])`
- (iv) `print ("python" [-5 : -1])`
- (v) `print ([2, 3, 4] [0 :] [2])`

```
t = np.array ( [0, 2, 5, 9, 14, 20, 27, 35] )
conc_inv = np.array ( [0.746, 1.128, 1.700,
2.463, 3.417, 4.562, 5.898, 7.424] )
```

- (b) Give the following pH metric titration data, employ the **forward finite difference** method to evaluate the first differential (equivalence point). 5

```
V_base = np.array ([1, 2, 3, 4, 5, 6 7])
```

```
pH = np. array ([0.1, 0.2, 0, 3, 3, 0.3, 0. 2,
0.1])
```

- (c) Write a Python program to find the product of two matrices, taking the matrices as input from the user. Any dimension of the matrices should not be less than 3 or more than. 5; if the dimensions exceed these limits, print an error message. 5

7. (a) Explain the below terms in one line each : 1×5=5

- (i) operand
- (ii) function
- (iii) token
- (iv) NameError
- (v) debugging

(b) For the below program :

```
for j in range (3, 6) :
```

```
for k in range (4, 7):
```

```
print (j*k)
```

(i) Write the output of the program

2

(ii) Convert the program so that it uses while loops instead of for loop.

3

(c) Write a program to print the sum of first n terms of the Taylor expansion of the sine function. Take n as input from the user.

Recall that $\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)!}$

5

8. (a) Answer any **two** of the below **4** parts :

$$2.5 \times 2 = 5$$

(i) Convert Hexadecimal XF34 to Octal base

(ii) Convert Octal 7143 to Binary base

(iii) Explain why Python is fast becoming the language of choice for scientific work

(iv) Explain how to set up the Python environment on a Windows PC from scratch.

(b) The below program will print 4 lines of output. Provide all 4 lines of output i = 0

5

```
def my_function (a=0, b = 3) :
```

```
i = 7
```

```
return i *a+b
```

```
print (my_function () )
```

```
print (my_function (1, 2) )
```

```
print (i)
```

```
i = 4
```

```
print (my_function (3) )
```

(c) The following is the kinetics data obtained from a second – order reaction. Plot the graph (inverse of the concentration of the reactant vs. time) in Python and perform a linear fit on the data. Print the slope, intercept, equation of the model and the correlation coefficient (R^2).