[This question paper contains 8 printed pages.]

Your Roll No.30/12/24

Sr. No. of Question Paper : 1056 **I**

Unique Paper Code : 2172013501

Name of the Paper : DSC: Inorganic Chemistry V – Basics of Organometallic Chemistry

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

Semester : V

Duration : 3 Hours Maximum Marks : 90

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt **six** questions.
3. **All** questions carry equal marks.

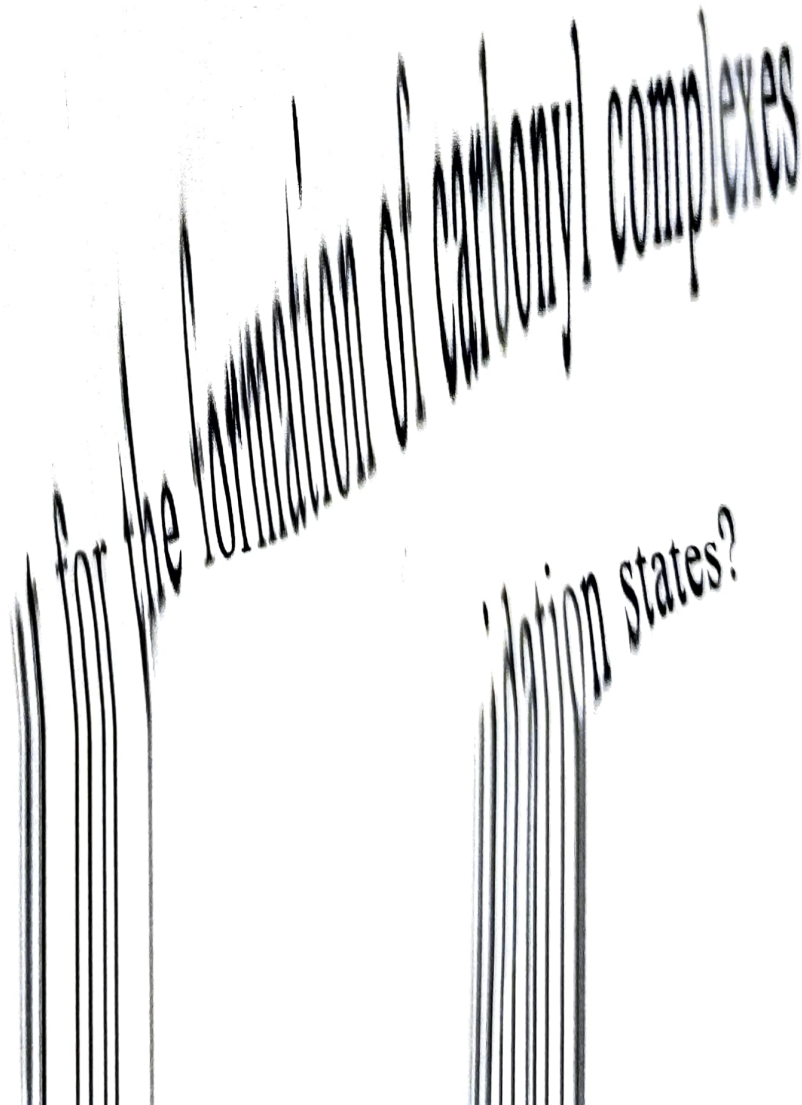
P.T.O.

1. (a) Define the following with suitable example :

(i) Organometallic compounds and its application

(ii) Hapticity. Give examples of ligands with hapticities of 3, 4 and 5.

(b) What is meant by Synergic effect? How does it



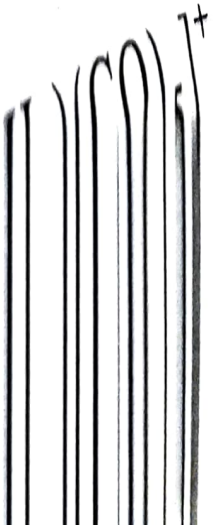
(c) What is Wilkinson's Catalyst? Explain its structure and how it is an effective homogenous catalyst for hydrogenation of alkenes. (5,5,5)

8. (a) Give two methods of synthesis of ferrocene and how does it react with the following :

(i) Butyl Lithium,

(ii) Formaldehyde and secondary amine.

(b) Predict whether the following obey the EAN rule :



(c) How to synthesized Zeise's salt? Discuss the bonding in Zeise's salt on the basis of Dewar-Chatt-Duncanson model. (5,5,5)

[This question paper contains 4 printed pages.]

19/12/19

Your Roll No.....

आपका अनुक्रमांक.....

Sr. No. of Question Paper : 1094 **I**

Unique Paper Code : 2172013502

Name of the Paper : DSC: Nucleic acids, Amino acids, Proteins and Enzymes

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

Semester : V

Duration : 2 Hours Maximum Marks : 60

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt four questions in all.
3. All questions carry equal marks.

1. a) How would you differentiate between Gly-Ala and Ala-Gly by Edman's degradation method? Write down the reactions involved.

b) How will you synthesize valine by Gabriels phthalimide method?

c) How will you differentiate between RNA and DNA by alkaline hydrolysis. Give mechanism of the reaction involved.

d) Write structure of NAD^+. Explain its role in an enzyme catalyzed reaction.

e) Discuss the effect of urea and heat on secondary structure of protein. (5x3)

2. a) The reaction of nonapeptide "A" with dansyl chloride gives dansyl derivative of Cysteine. Peptide "A" on reaction with cyanogen bromide gives tripeptide containing Cys, Met, Lys and hexapeptide containing Try, Gly, Ala, Phe, Leu and Asp. Partial hydrolysis of "A" yields Lys-Met-Leu, Ala-Gly-Try, Cys-Lys, Leu-Phe-Ala, Gly-Try-Asp and Met-Leu- Phe. Deduce the structure of "A".

Give all the reactions involved. Write down the products obtained when B is treated with Carboxypeptidase and Chymotrypsin.

b) What are the structures of lysine at pH = 1.5, 3.2, 9.74 and 12? To which electrode does lysine

migrate at each pH? Which of the structure will be present at isoelectric point? (10,5)

3. a) Name the monomers used in preparation of resin used in Solid Phase Merrifield method. How would you synthesize a tripeptide Leu-Ala-Lys by this method? Give its advantages over general method of synthesis.

b) Discuss the following about the Trypsin:

i. Specificity

ii. Catalytic Triad

iii. Pocket at the active site

c) Explain the various types of forces that are responsible for the stabilization of tertiary structures of proteins. (6,6,3)

4. a) Discuss the different types of reversible enzyme inhibition with examples.

b) Explain different classes of enzymes with one example each.

c) What do you understand by K_m in an enzymatic reaction? Discuss its significance. (6,6,3)

5. a) Write the structures showing the hydrogen bonding between the following nucleotide base pairs:

   i. Thymine and Adenine

   ii Guanine and Cytosine

   b) Write short note on the types of RNA and their biological functions.

   c) Discuss the different steps involved in DNA Replication. (5,5,5)

6. Write down short notes on any three of the following:

   a) Electrophoresis

   b) Ninhydrin test

   c) Genetic code

   d) Factors affecting the enzyme activity (5,5,5)

[This question paper contains 4 printed pages.] 16/12/24

Your Roll No.....

आपका अनुक्रमांक.....

Sr. No. of Question Paper : 5824 **I**

Unique Paper Code : 32171501

Name of the Paper : DSC (Organic Chemistry-IV) Biomolecules

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

Semester : V

Duration : 3 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt Six questions. All parts of a question should be attempted together.
3. Each question carries 12.5 marks.

1. (a) List any two reactions that were not explained by the open chain structure of glucose. How does the cyclic hemiacetal structure of glucose explain them.

P.T.O.

(b) What is iodine number? What is it significance?

(c) Give the complete name and structure of dAMP and UDP

(4.5, 4, 4)

2 (a) Which form of alanine would you expect to predominate under (i) Strongly acidic solution (ii) Strongly basic solution (iii) At its isoelectric point. Indicate which part of the dipolar ion behaves as a potential acid or potential basc and also find out the isoelectric point of alanine (pKal=2.3, pKa2 = 9.7)

(b) How will you convert:

(i) D-glucose to the D-arabinose

(ii) D-glucose to D-fructose

(c) Discuss the secondary structure of proteins.

(4.5, 4, 4)

3. (a) Explain, why D-glucose and D-fructose give the same osazone? Give the mechanism of osazone formation for D-glucose.

(b) Draw the complementary DNA sequence of the given fragment specifying the direction 5-ATGC-3

(c) Explain the term rancidity of oils and fats. How many types of rancidity occur in oils and fats? Discuss.

(4.5, 4, 4)

4. (a) Differentiate between nucleosides and nucleotides? Give the structure of guanosine-5'- triphosphate.

(b) Write down the reaction of glucose with (i) HNO_3 (ii) HIO_4

(c) Provide the full form and structure of ATP Explain, why ATP is called the universal currency of cellular energy. (4.5, 4, 4)

5. (a) How will you synthesize the dipeptide Gly-Val using Merrifield resin. Discuss its advantages over other methods?

(b) Differentiate between competitive and non competitive enzyme inhibition using suitable examples.

(c) List four important characteristics of Watson and Crick model of DNA. (4.5, 4, 4)

6. (a) What is fermentation? Write down the fate of pyruvate in alcoholic and lactate fermentation with enzymes involved.

(b) Explain Dansyl Chloride method of N-terminal analysis. What is the advantage of this method over other methods of N-terminal analysis?

(c) Discuss replication of DNA. (4.5, 4, 4)

7. (a) A pentapeptide A having empirical composition Lys, Phe, Thr, Leu, Asp gave DNP-Thr on treatment with DNFB followed by hydrolysis. Treatment of A with carboxypeptidase released Asp. Treatment of A with trypsin gave a tripeptide, (Lys, Leu, Thr) and a dipeptide (Asp, Phe). Elucidate the sequence of amino acids in A.

(b) Write down three irreversible steps in the glycolysis process. Write all the structures and the name of enzymes involved.

(c) Give the synthesis of proline by phthalimide malonic ester method. (4.5, 4, 4)

8. (a) Define saponification value and give its significance. Calculate the saponification value of glyceryl tripalmitate having molecular weight 806 (molecular weight of KOH= 56).

(b) Write short notes on any two of the following:

(i) Genetic code

(ii) Reversion and rancidity

(c) Using Haworth projection draw the structures of the following:

(i) α-D-Glucopyranosyl-β-D-fructofuranoside

(ii) 4-O-(β-D-Galactopyranosyl)-α-D-Glucopyranose (4.5, 4, 4)

[This question paper contains 8 printed pages.]

23/12/24

Your Roll No.....

Sr. No. of Question Paper : 5930 **I**

Unique Paper Code : 32177902

Name of the Paper : Elective Discipline Specific-1: Inorganic Materials of Industrial Importance

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

Semester : V

Duration : 3 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll. No. on the top immediately on receipt of this question paper.

2. Attempt **SIX** questions in all.

3. **Question 1** is compulsory.

4. Attempt **any five** other questions.

P.T.O.

1. (a) Fill in the blanks/Write True or False as required:

(i) A secondary battery cannot be recharged and should be discarded after single use. (True/False).

(ii) The shorter the annealing period, the more durable the glass article. (True/False)

(iii) _____ is the process of transformation of a molten mass of material into a non-crystalline, amorphous and transparent solid.

(iv) A _____ cell converts fuel directly into electricity without combustion.

(v) Bronze is a metal alloy that is primarily made of _____

(vi) Safety glass has a layer of _____ sandwiched between two layers of glass.

(vii) Urea is an example of _____ fertilizer.

(viii) The additives used in paint formulation which prevent excessive foam formation during manufacturing are called as _____ .

(ix) The process of surface hardening caused due to diffusion of boron into the base metal or alloy is called _____ .

(b) Give one word for the following:

(i) Full form of MAP

(ii) A paint which can withstand high working temperature

(iii) Nutrients which are required in very small amounts by plants

(iv) The process of applying a protective zinc coating to iron or steel

(v) Fibrous glass composed of intermingled fine threads or filaments of glass (10,5)

2. (a) What is a battery? Differentiate between primary and secondary batteries.

(b) Explain briefly the principle, working and applications of lithium ion battery

(c) How do photons initiate the reactions in a solar cell? What are the advantages of a solar cell? (4, 4, 4)

3. (a) How does urea function as an effective fertilizer for plants? Give one method for the manufacturing of urea.

(b) What are superphosphates of lime? Explain any one method of its preparation

(c) What are composite materials. Discuss their important applications. (4, 4, 4)

4. (a) Discuss the importance of 'annealing' in the manufacturing of glass

(b) Briefly describe the formation, characteristics and applications of carbon fibers

(c) Discuss the composition, properties and applications of alloys of aluminium. (4, 4, 4)

5930

5. (a) What are superconductors? Discuss any three applications of superconductors

(b) Write down the uses of ceramic products. How is glazing of ceramics done?

(c) What are thermosets and thermoplastics? Explain giving examples in each case. (4, 4, 4)

6 (a) How does a flame retardant paint work? Mention the functions of the following additives in a paint formulation.

(i) Plasticizers

(ii) Anti-skinning agents

(b) What is the difference between electroplating and electroless plating. How electroless plating is more beneficial over electroplating.

(c) Differentiate between drying oils and semi-drying oils. (4, 4, 4)

7 (a) What are the causes of failure of a paint film? How can it be prevented?

(b) Why is it necessary to add a retardant to the cement? Give an example of a retardant and explain with chemical reactions how it functions in retarding the setting of cement

(c) State the alloying elements added to steel to get alloy steels and the effect they produce. Give at least one example of each. (4, 4, 4)

8 (a) What are mixed fertilizers? Explain the advantages and disadvantages of mixed fertilizers.

(b) Differentiate between Sheradizing and Chromising.

(c) What are the advantages and disadvantages of a lead acid battery.

(4, 4, 4)

[This question paper contains 8 printed pages.]

19/12/24

Your Roll No.....

Sr. No. of Question Paper : 5878 **I**

Unique Paper Code : 32171502

Name of the Paper : DSC-Physical Chemistry V: Quantum Chemistry & Spectroscopy

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

Semester : V

Duration : 3 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll. No. on the top immediately on receipt of this question paper.

2. Attempt 3 questions from Section A and 3 questions from SectionB. A total of 6 questions to be attempted.

3. Please indicate the section you are attempting at the appropriate place and do notintermixthesections. The questions should be number edinaccordance to the number in the question paper.

P.T.O.

4. Calculators and log tables may beused.

Physical Constants

Planck's constant 6.626×10^{-34} JS

Velocity of light 3×10^{8} m/s

Atomic mass unit 1.661×10^{-27}; kg

Avagadro's number 6.023×10^{23} mol^{-1}

Mass of electron 9.109×10^{-31} kg

SECTION A

Attempt **any 3** questions from this section

1. (a) Explain the following terms:

(i) Linear operator

(ii) Laplacian operator

(iii) Hamiltonain operator.

(b) Draw the Ψ and Ψ^2 patterns for various levels of the Simple Harmonic Oscillator. What conclusions can be drawn from these patterns?

(c) Write short notes on any two of the following:

(i) Bohr correspondence principle

(ii) Heisenberg Uncertainty Principle

(iii) Rigid rotator approximation (4.5,4,4)

2. (a) Indicate which of the following will lead to an eigen value equation. Report the eigen value, if any.

(i) $\frac{d}{dx}\exp(i\omega x)$

(ii) $\frac{d^2}{dx^2}(\sin 3x)$

(iii) $\frac{d^2}{dx^2}(5x^2)$

(b) Giving reason, state which of the following are acceptable wave functions in the indicated interval:

(i) sin x $(0,2\pi)$

(ii) e^{-x} $(-\infty, \infty)$

(c) Calculate the wavelength in nm, for the transition from HOMO to LUMO in 1, 3 butadiene molecule. The C-C and C = C bond lengths are 154pm and 135pm respectively. (4.5,4,4)

3. (a) For a particle of mass 'm' in a cube of edge length 'a', the energy of a quantum level is found to be $17\ h^2/(8ma^2)$. What are the quantum numbers and the degeneracy of the level?

(b) Show that two eigen functions of a Hermitian operator having different eigen values are orthogonal to each other.

(c) A particle of mass 'm' is confined to a one-dimensional box with the origin at centre of the box. The box extends from -a/2 to +a/2. The potential energy function V(x) is V(x) = 0 (inside) and $V(x) = \infty$ (outside). (4.5,4,4)

Write the Schrodinger equation for the system showing separate equation inside and outside the box. (4.5,4,4)

4. (a) Write the Schrodinger wave equation for hydrogen atom in polar coordinates while giving the significance of the terms involved.

(b) What do you understand by the commutation between two operators?

Show that position and linear momentum operator do not commute with each other.

(c) Why do we need to employ approximate methods to determine solution for multi- electron atoms? Explain Variation principle as an approximate method to determine approximate wave function.

(4.5,4,4)

SECTION B

Attempt any 3 questions from this section

5. (a) Briefly explain Rule of Mutual exclusion and its role in structure elucidation.

(b) Explain the different modes of vibration in the following two polyatomic molecules:water and carbon dioxide. Are they both IR and Raman active? Explain your answer.

(c) The rotational spectrum of $^{79}Br\ ^{19}F$ shows a series of equidistant lines 0.71433 cm^{-1} apart. Calculate the rotational constant B, the moment of inertia and bond length of the molecule. (4.5,4,4)

6. (a) What is Raman effect? Explain the origin of Stokes and Anti-Stokes line.

(b) Which of the following molecules will give rise to observable rotational and vibrational spectra HCl, N_2, CO, H_2O? Explain giving reasons.

(c) The $^1H^{35}Cl$ molecule shows pure rotational lines at the following frequencies (cm^{-1}) 20.7, 41.5, 62.0, 83.0, 103.8.

(i) Assign the lines to the rotational transitions, $J \rightarrow J+1$.

(ii) Calculate the bond distance of HCl.

(m_H =1.673 × 10^{-27}kg, m_{Cl} =58.06 × 10^{-27}kg)

(4.5,4,4)

7. (a) What is the effect on the microwave spectrum of $C^{16}O$ if $^{16}0$ is substituted by ^{18}O?

(b) Calculate the number of translational, rotational and vibrational degrees of freedom for

(i) CO_2

(ii) H_2O

(iii) Benzene

(iv) CH_4

(c) The force constant for $'H'^{9}F$ is 966 N^{-1}. Calculate:

(i) The zero-point vibrational energy of this molecule when it follows harmonic motion.

(ii) The frequency of the electromagnetic radiation

to excite this molecule from the ground state to the first excited state. (4.5,4,4)

8. (a) Indicate with the help of the Jablonski diagram, the various processes by which the excited electronic states get deactivated. What is the difference between fluorescence and phosphorescence?

(b) Arrange the following groups in increasing order of their absorption frequencies: Give justification

(i) CF, CCI, CBr, CH

(ii) C-C, C=C, C≡C

(c) What are the characteristics of TMS which make it useful as a reference in NMR spectrum? (4.5,4,4)

01/01/2025

[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 : $1\times5=5$

(i) NUMPY

(ii) HDD

(iii) AI

(iv) DOS

(v) ALU

(b) Write the below algebraic/scientific expressions in Python friendly format : $1\times=5$

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

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

(iii) $(2 + 3i)$

(iv) $RT\,lnK$

(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 : 1×5=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 $\int_{5}^{10}\left(x^2-3x+2\right)dx$ 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 : "H", 2 : "He", 3 : "Li",....., 11.8:" 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 : "He", 10 : "Ne", 18 : "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 : $1 \times 5 = 5$

(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 : $2.5 \times 2 = 5$

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])

(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 : 2.5×2=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 coefficient (R^2). 5

```
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] )
```

***

[This question paper contains 8 printed pages.] 26/12/24

Your Roll No.....

Sr. No. of Question Paper : 6046 I

Unique Paper Code : 32177908

Name of the Paper : DSE: Green Chemistry

Name of the Course : **BSc. (H) Chemistry, BSc. (Prog) Analytical Chemistry/ Industrial Chemistry**

Semester : V

Duration : 3 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll. No. on the top immediately on receipt of this question paper.
2. Attempt **any six** questions. **First question is compulsory.**
3. **All** questions carry equal marks.
4. Attempt all parts of a question together.
5. Take molecular mass of C = 12, N = 14, O= 16, S = 32, H = 1

P.T.O.

1. (i) (a) Which of the following are among the 12 principles of Green Chemistry?

(a) Design commercially viable products

(b) Use only new solvents

(c) Use catalysts, not stoichiometric reagents

(d) Re-use waste

(ii) Green chemistry is more expensive than traditional chemistry?

(a) True

(b) False

(iii) The term which refers to the breakup within a compound due to microbial activity is?

(a) Microbial degradation

(b) Agro-degradation

(c) Photo-degradation

(d) Decomposition

(iv) What is the U.S. Presidential Green Chemistry Challenge Award?

(a) An award related to recycling

(b) An award for industry only

(c) The only chemistry award given by the President

(d) Challenges companies to become fuel efficient

(b) Fill in the blanks with the appropriate word:

(i) Benzene, a _____ substance, is an important industrial solvent used in the production of pharmaceuticals, plastics, and dyes?

(ii) _____ is an excellent 'green' solvent as well as a greenhouse gas?

(iii) _____ was a co-founder of the worldwide green chemistry movement and the first director of the Green Chemistry Institute, now part of ACS?

(iv) _____ is fulfilling the needs of the present generation without compromising the ability of future generations to meet their needs?

(c) What do you mean by supercritical carbon dioxide?

Discuss the chemistry of cleaning action of surfactant assisted supercritical CO_2.

(4, 4, 4.5)

2. (a) Define green chemistry. Discuss some important environmental laws that leads to green chemistry.

(b) Elaborate in detail the limitations in pursuing the green chemistry.

(c) Define the role of green chemistry in sustainable development? (4, 4, 4.5)

3. Give the Green Synthesis of following compounds:

(a) Catechol

(b) Adipic Acid

(c) Citral

(d) Methyl methacrylate

(e) Furfural

(2.5 × 5)

4. (a) What are the problems associated with inorganic pigments and organic dyes? How these problems can be solved?

(b) Explain the efficient green synthesis of plastic made from corn

(c) Sonochemical Simmons-Smith reaction is a better alternative to conventional method Elaborate.

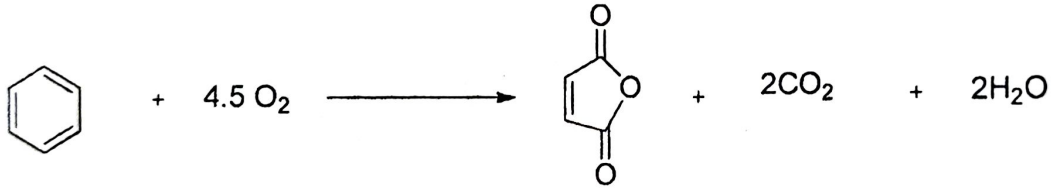
(4, 4, 4.5)

5. (a) What do you mean by supercritical carbon dioxide? Discuss the chemistry of cleaning action of surfactant assisted supercritical CO_2. 6

(b) How % yield is different from atom economy. Discuss any one reaction where % yield is 100% but not the atom economy.

(c) Calculate the atom economy of the following reactions:

(Mol mass: C=12, H=1, O=16, Br=80)



(ii)

(4, 4.5, 4)

6. Discuss the following microwave assisted reactions.

(a) Hofmann elimination reaction

(b) Oxidation of Alcohol

(c) Decarboxylation

(4, 4.5, 4)

7. (a) Explain the enzymatic inter-esterification reaction for the production of healthier fats and oils.

(b) Discuss briefly the limitations of tin based marine anti-foulant. How are they overcome using environmentally safe anti-foulant?

(c) Explain how cradle to cradle recycling concept is applied to carpets? (4, 4.5, 4)

8. (a) Give chemical reaction for solvent free synthesis of azomethine in the laboratory. What are its advantages over conventional methods?

(b) Compare heterogeneous and homogeneous catalysis in terms of green chemistry.

(c) What are biocatalysts? What are the advantages of bio-catalytic conversions? Give one example of the reaction. (4, 4, 4.5)

[This question paper contains 8 printed pages.] 24/12/24

Your Roll No.....

Sr. No. of Question Paper : 1113 **I**

Unique Paper Code : 2172013503

Name of the Paper : Quantum Chemistry and Covalent Bonding

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

Semester : V

Duration : 3 Hours Maximum Marks : 90

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt only **six** questions out of **eight**.
3. Use of scientific calculators and Logarithmic tables is allowed.
4. Attempt all parts of a question together.

P.T.O.

Physical Constants

Planck 's constant	6.626×10^{-34} J s
Velocity of Light	3×10^{8} ms^{-1}
Avogadro's Number	6.022×10^{23} mol^{-1}
Mass of Electron	9.1×10^{-31} kg
Boltzmann Constant	1.38×10^{-23} J K^{-1}

1. (a) A particle of mass m, in a one-dimensional box of length a can be represented by the function, $\psi(x) = \sin\frac{n\pi x}{a}$ (n=1,2,3...). Normalize the given function $\psi(x)$ and find whether it is an eigen function of (i) p_x (ii) p_x^2.

(b) Write four properties of a function to make it acceptable as a solution of Schrodinger equation. Determine whether the following functions are acceptable or not acceptable as state functions over the interval indicated, giving appropriate reasons.

Function	Interval
$(1-x^2)^{-1}$	$(-1,+1)$
$exp(-x)$	$(0,\infty)$

(c) Evaluate the commutator $[\widehat{L_x},\widehat{L_y}]$ where $\widehat{L_x}$ and $\widehat{L_y}$, are the angular momentum operators along the x and y-direction respectively. (5,5,5)

2. (a) Are the following functions eigen functions of the operator $\frac{\widehat{d^2}}{dx^2}$? If so, give the eigen value.

(i) $f(x) = \exp\left(-\frac{x^2}{2}\right)$

(ii) $\cos 2x$

(b) Consider a particle of mass 'm' in a cubic box of edge length 'L'. What is the degeneracy of the level that has energy three times the lowest energy ? Write the mathematical expressions for the degenerate wavefunctions.

P.T.O.

(c) If A and B are two atoms bonding along the z-axis predict, giving reasons, which of the following atomic orbitals can combine:

(i) φ_{2s}^{A} and $\varphi_{2p_z}^{B}$

(ii) φ_{1s}^{A} and φ_{2s}^{B}

(iii) $\varphi_{2p_x}^{A}$ and φ_{2s}^{B} (5,5,5)

3. (a) Write the expression for the Hamiltonian operator for the helium atom explaining briefly all the terms involved. Simplify this expression using the Bom Oppenheimer approximation. Write the expression for the corresponding Schrodinger's equation.

(b) Evaluate the expectation value of the radius, (r), at which the electron in the ground state of Hydrogen atom (Z=1) is found. Given the wave function for this state is

$\psi_{1,0,0} = \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} \exp\left(-\frac{zr}{a_0}\right)$ where a_0 is the Bohr radius and $\int_0^\infty r^n \exp(-ar)\, dr = \frac{n!}{a^{(n+1)}}$.

(c) Write the electronic configuration of H_2, H_2^+ and hypothetical H_2^- species using molecular orbital theory. Explain why He_2^+ exist whereas He_2 does not. (5,5,5)

4. (a) A diatomic molecule can be treated as a simple quantum mechanical oscillator. How is the simple Schrodinger Wave Equation (SWE) modified for this system? Show that

(i) $\exp(-\beta x^2)$ is a solution to this SWE and

(ii) $E = \frac{1}{4\pi}\sqrt{\frac{k}{\mu}}$, here k is the force constant and μ is the reduced mass)

(b) What is the degeneracy of each of the following energy levels of H atom?

(i) $\frac{-e^2}{72\pi\epsilon_0 a_0}$ (ii) $\frac{-e^2}{128\pi\epsilon_0 a_0}$

(c) Explain and calculate zero point energy (ZPE) of an electron in a one dimensional box of infinite height and 1 Å length. State the Bohr's Correspondence principle. (5,5,5)

5. (a) Show that the wave functions describing the 1s atomic orbital and the 2s atomic orbital for the hydrogen atom are orthogonal. Given that

$$\psi_{1s} = (\pi a_0^3)^{-1/2} \exp(-r/a_0) \text{ and}$$

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \{2 - (r/a_0)\} \exp\left(\frac{-r}{2a_0}\right)$$

where a_0 is Bohr's radius and

$$\int_0^\infty r^n \exp(-ar)\, dr = n!/a^{(n+1)}.$$

(b) Set up the Hamiltonian operator for a particle oscillating about a mean position (a simple harmonic oscillator). Explain the significance of zero-point energy of a simple harmonic oscillator.

(c) Why the quantum number 'n' cannot be assigned a zero value while solving for the particle in a 1-D box? Give the units of ψ^2 for a particle in a 1-D box. (5,5,5)

6. (a) A particle of mass m exists in a one-dimensional box of length L. Using the trial wave function $\Psi_{trial} = Nx(L - x)$ evaluate the energy associated with the lowest energy level and comment on whether this trial wave function is an acceptable function according to the variation theorem.

(b) Show that operators corresponding to $\hat{x}$ and $\hat{p}_x$ do not commute. Give the physical significance of your result.

(c) What do you understand by Hermitian operators? Prove that all the eigen values of Hermitian operators are real numbers. (5,5,5)

7. (a) Write the LCAO-MO trial wave function of H_2^+, using Molecular Orbital approach. Derive the expressions for molecular orbital wave functions corresponding to the bonding and anti-bonding energy levels of H_2^+.

(b) Plot the radial probability distribution functions for an electron in hydrogen atom where $n = 1$ and $n = 2$. Explain the plots briefly.

(c) Explain the significance of orthonormality principle giving relevant mathematical expressions. (5,5,5)

8. Write short notes on **any three** :

(a) Postulates of Quantum Mechanics

(b) Pauli's Exclusion principle (quantum mechanical approach)

(c) Configuration Interaction

(d) Variation Theorem

(5,5,5)