Unique Paper Code: 32171101_OC

Name of the Paper: Inorganic Chemistry I

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

Semester: I

Duration: 3 hours **Maximum Marks:** 75

Instructions for Candidates:

Attempt any four QUESTIONS in all.

All Questions carry equal marks

The questions should be numbered in accordance with the number in the question paper.

Calculators and log tables may be used.

1. a) What do you mean by quantum numbers? Name different types of quantum numbers and their significance.
   b) Give Allred and Rochow's scale of electronegativity. Calculate the electronegativity of silicon atom using this scale. The covalent radius of Si atom is 1.175 Å.
   c) State the Pauli Exclusion Principle. How can this principle be used to fix the maximum capacity of the various energy levels in an atom?
   d) Explain the trends in variation of valency in groups and periods of s and p block of elements.
   e) Explain why the melting point of NaCl is higher than that of $AlCl_3$?

(5,4,4,3,2.75)

2. a) What are Slater rules? Using Slater's Rules calculate Z* for the following elements:
      i) 4s electron in Ca
      ii) 4s electron in Sc
      iii) 3d electron in Sc

   b) Which sets of quantum numbers are not possible and why?

      i) n = 5, l=4 m=0, ms = ½
      ii) n =3, l=0, m =-1, ms = -1/2
      iii) n=3, l=1, m =2, ms = ½
      iv) n =2, l =2, m =0, ms =1/2

   c) What is radius ratio? How can it help to predict the structure of an ionic compound? What are its limitations?
   d) What do you understand by equivalent and non-equivalent hybrid orbitals? Give one example of each.
   e) What is Hund's rule of maximum multiplicity?

(5,4,4,3,2.75)

3. a) Derive the Schrodinger wave equation for H-atom starting with simple sine wave equation. Explain all the term associated with it.
   b) Draw the MO energy level diagram for N_2^+. Discuss its bond order and magnetic

behaviour. Why is the bond order in N_2^+ less than in N_2, molecule?

c) Using Pauling's method, calculate the radii of Na^+ and F^- ions. The observed internuclear distance in NaF crystal is 213 pm.

d) Define electronegativity. How the electronegativity (varies with s-character in different hybridisation of organic compounds?

e) Explain why properties of lithium resembles with those of magnesium?

(5,4,4,3,2.75)

4. a) Derive Born-Lande equation for lattice energy.

b) What is radial node? Calculate the number of radial nodes for 3s, 2p, 4d, and 5f orbitals.

c) What are isoelectronic ions? How effective nuclear charge affects the radii of isoelectronic ions: N^{3-}, O^{2-}, F^-, Na^+, Mg^{2+}?

d) Give trends in melting point and hardness for the

i) LiCl and SrO and

ii) NaCl and BaO

e) Differentiate between Frankel and Schotkey defects.

(5,4,4,3,2.75)

5. a) Explain the terms polarization, polarizing power and polarizability. State giving reason, which cation will have greater polarizing power in the following:

i) Na^+ or Mg^{2+}

ii) Pb^{2+} or Pb^{4+}

b) Calculate the value of Madelung constant A for MgO with given data r_0 = 2.10 Å, n =7, N= 6.02 X 10^{23} , U_0 = -3940 KJ/mole, e = 4.8 X 10^{-10} esu.

c) Both, NH_3 and H_2O molecules are formed by SP^3 hybridization but the bond angles are different. Explain on the basis of VSEPR theory.

d) Explain why:

i) Density of ice is less than that of water.

ii) o-nitrophenol is less soluble in water than p-nitrophenol

e) Which of the elements Na, Mg, Si & P will have the greatest difference between the first and second ionisation enthalpy? Explain.

(5,4,4,3,2.75)

6. a) Write a note on Band theory of metallic bonding.

b) The internuclear distance in HI is 1.62 Å. Assuming complete transfer of electron from H to I, calculate dipole moment of HI. If the measured dipole moment is 0.38 D, calculate the % ionic character of HI. Given e = electronic charge = 4.8 X 10^{10} e.s.u.

c) Give the shape and hybridization of following molecules or ions:

i) PCl_3

ii) ICl_2^-

iii)ClF_3

iv)PCl_6^-

d) Explain why orbitals like 1p, 2d and 3f are not possible?

e) Write a note on Bent's Rule.

(5,4,4,3,2.75)

32175915 III Set A Solution, Conductance, Electrochemistry and Functional Group Generic Elective

Unique Paper Code	: 32175915_OC
Name of the Paper	: GE-3: Solutions, Phase Equilibrium, conductance, Electrochemistry and Functional Group Organic Chemistry-II
Name of Course	: B. Sc. (Hons.)
Semester	: I / III
Duration	: 3 hours
Maximum Marks	: 75

Instructions for Candidates:

- Use separate answer sheets for **Section – A** and **Section – B** and upload separately.
- Both sections carry equal marks.
- Attempt **four** questions in all, **two** questions from each section.
- Each question carry **18.75** marks.

Section A: Physical Chemistry

(Attempt any two questions)

Q. 1

a) State Nernst distribution law. Give conditions under which it is valid. Also write its application.

b) What are azeotropes? Give its example. Is it possible to separate the components of an azeotropic mixture by simple distillation? Explain

c) Define congruent point. Justify the statement that it is an invariant point. Draw and discuss a well-labelled phase diagram of $FeCl_3$-H_2O system.

d) Define critical solution temperature (CST). Give degree of freedom at CST and under the curve. Explain the effect of addition of sodium chloride and succinic acid on CST of water-phenol system with well labelled diagram.

(3.75, 3, 6, 6)

Q. 2

a) State and explain Kohlrausch's law of independent migration of ions. Also, explain the variation of specific conductance, molar and equivalent conductance at infinite dilution of weak and strong electrolytes with suitable graph.

b) Give the principle of potentiometric titration. Also give the advantages of potentiometric titration over volumetric titrations using indicators. Why do we prefer potentiometer for the measurement of EMF of a cell over voltmeter?

c) Transport number of Na^+ is 0.463 (dilute solution of NaCl in methanol). Calculate transport number for H^+ (dilute solution of HCl in methanol) if Λ^∞ for (NaCl in methanol) is 96.9 $ohm^{-1}cm^2mol^{-1}$ and Λ^∞ for (HCl in methanol) is 192 $ohm^{-1}cm^2mol^{-1}$ respectively.

d) 100 g each of ethanol and methanol are mixed at 20ºC to prepare an ideal binary mixture. The vapour pressure of pure methanol is 88.7 mm Hg and that of pure ethanol is 44.5 mm Hg at 20ºC. Calculate (i) total vapour pressure of the solution, (ii) partial vapour pressures of ethanol and methanol and composition of the vapour phase.

(6, 6, 3, 3.75)

Q. 3

a) Write the thermodynamic criteria of phase equilibrium of a system and also drive the mathematical expression of Gibbs phase rule at constant pressure for a reactive and non-reactive system.

b) Differentiate between reversible and irreversible electrochemical cells giving examples.

c) An electrochemical cell consist of two half-cell reaction as

$$AgCl(s) + e^- \longrightarrow Ag(s) + Cl^-(aq)$$
$$Cu(s) \longrightarrow Cu^{2+} + Cl^-$$

Calculate the mass of copper deposited on passing 0.5A current for 1 hour.

d) What is salt bridge? Write its functions emphasizing on its role in eliminating the liquid junction potential in an electrochemical cell.

e) Derive the expression to determine the pH value of an unknown solution by using hydrogen electrode with well labelled diagram.

(5, 2, 3, 3.75, 5)

Section B: Organic Chemistry

(Attempt any two questions)

Q.4

a) How can a mixture of arginine and aspartic acid be separated by electrophoresis using a buffer solution having a pH=6.0?

b) Outline the chemistry of Hinsberg test?

c) How ethylacetoacetate is synthesized using Claisen condensation? Give the mechanism.

d) Write short note on the following:
   i) Secondary structures of proteins
   ii) Hell-Volhard-Zelinsky reaction.

e) Explain why D-fructose reduces Fehling's solution although it is a ketohexose.

(3, 3, 3, 5, 4.75)

Q.5

a) Give a detailed account of Hofmann elimination and compare it with Satyzeff Elimination.

b) What is mutarotation? Give its mechanism using α-D-glucopyranose as an example.

c) Giving reasons, arrange the following in order of their increasing basicity: o-nitroaniline, m-nitroaniline and p-nitroaniline.

d) Convert:

i. Phenylacetic acid to Benzylamine
ii. Aniline to p-bromoaniline

e) Explain Edman degradation method for the determination of N-terminal amino acid of peptide.

f) How do maltose and cellobiose differ in their structures?

(3, 3, 3, 4, 3.75, 2)

Q. 6

a) Synthesize dipeptide ala-val by using t-BOC &DCC. Give the name and structure of protecting and activating groups.

b) Complete the following reaction and predict the structure of compounds A,B,C,D

i) $C_6H_5CHO + (CH_3CO)_2O \rightarrow A+B$

ii) $BrCH_2COOC_2H_5 + CH_3COCH_3 \xrightarrow{Zinc} C$

iii) $C_6H_5NH_2 + C_6H_5COCl \xrightarrow{NaOH} D$

c) Discuss the basicity order of the following and arrange them in order of increasing basic strength.

$C_6H_5NH_2$, $C_6H_5NHCH_3$, CH_3NH_2, $CH_3CH_2NH_2$

d) How will you convert D-arabinose to D-glucose and D-mannose.

e) Give suitable explanation, arrange the following in increasing order of their reactivity with phenol: Acetyl Chloride, Acetamide, Methyl acetate

(4.75, 4, 4, 3, 3)

Unique Paper Code : 32171102

Name of Paper : Chemistry C-II Physical Chemistry I

States of Matter and Ionic Equilibrium

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

Semester : I

Duration : 3 hours

Maximum Marks : 75

Instructions for candidates

1. Do any **four** out of the six questions given.
2. Answer all the parts of a question together.
3. Label clearly the number of question.

1. a)At moderate pressure a real gas occupies less volume than an ideal gas. True or False? Give reason.

b) The boiling point of a liquid is 350K and its heat of vaporization is 85kJmol^{-1}. Calculate the temperature at which the liquid will boil if the pressure is 2.6 x 10^{3}Nm^{-2}.

c) A substance of atomic weight 63 crystallizes in an fcc lattice of unit cell edge length 350pm. Predict the first four lines of the X ray diffraction pattern using X rays of wavelength 154pm. Index the lines.

d) A solution of CH_3COOH and CH_3COONa acts as a buffer but a solution of HCl and NaCl does not. Explain.

(3.75, 5, 5, 5)

2. a) Why are bubbles formed more easily in soap solution than in water?

b) At what pressure does the mean free path of helium gas at 25^{o}C becomes equal to the diameter of the atom itself. The volume of a helium atom is 2.784 x10 $^{-30}$ m^{3}.

c) Calculate the solubility of AgCN in a buffer of pH 3, given solubility product of AgCN is1.2x 10 $^{-16}$ and ionisation constant for HCN is 4.8 x 10 $^{-10}$.

d) List the symmetry elements present in an ammonia molecule? Illustrate diagrammatically.

(3.75, 5, 5, 5)

3. a) Explain why phenolphthalein cannot be used as an indicator in titration of strong acid and weak base.

b) A substance having tetra atomic molecules has a molar heat capacity $C_{v,m}$ of $79JK^{-1}mol^{-1}$at 500K.

(i) Predict its geometry
(ii) How many modes of vibrational motion does it have?
(iii) What will be its molar heat capacity $C_{v,m}$ at room temperature?

c) If 50 mL of 0.2 M CH_3COOH (ionization constant = 1.8×10^{-5}) is being titrated with 0.1 M NaOH. What is the pH of the solution when:

(i) 0 mL of NaOH is added
(ii) 10 mL of NaOH has been added.
(iii) 50 mL of NaOH has been added.

d) Calculate the Miller indices of the faces having the following intercepts

(i) 2a,3b,4c
(ii) -2a, b, 3c
(iii) 1/2a,2b,∞ c
(iv) 3/2a,2b,c
(v) 5/2a,5/2b,c

(3.75, 5, 5, 5)

4. a) Viscosity of liquids decreases as temperature is increased but that of gases increases. Explain

b) State whether the following statement is correct giving reason. If the statement is incorrect correct it giving reason.
If a little HCl is added to water the concentration of H^+ ions changes causing the ionic product of water to change.

c) The radius of Fe atom is 1.24Å. It occurs both in fcc and in bcc forms. Calculate density of each.

d) Calculate the mass of solid CH_3COONa that must be dissolved in 250 cm^3 of 0.09M CH_3COOH (K^o_a is $1.8X10^{-5}$)in order to give a solution of pH 4.7

(3.75, 5, 5, 5)

5. a) Explain why the position of H atoms in a crystal of sugar cannot be deduced from its X ray diffraction pattern.

b) Calculate the value of σ, λ, Z_1 and Z_{11} for N_2 molecules at 25°C and 10^{-3} torr given b = $39.1 cm^3 mol^{-1}$.

c) The solubility of Ag_2CrO_4 is 0.001g/L. Calculate its solubility product. What will be its solubility in a solution containing10g/L of K_2CrO_4?

d) Write the virial equation for a real gas. What are the advantages of using this equation as compared to the van der Waals equation?

(3.75, 5, 5, 5)

6. a) Why are x rays always used for studying crystal structures? Can any other rays be used instead of x rays? Why?

b) The compressibility factor for 1 mole of van der Waal's gas at 0 °C and 100 atm is found to be 0.5. Assuming that the volume of gas molecules is negligible, calculate the van der Waal's constant **a**.

c) On passing H_2S, CoS precipitates in basic solution but CuS precipitates in acidic medium. Explain

d) Calculate the degree of hydrolysis of ammonium acetate in a solution of concentration 0.05M. Also calculate the hydrolysis constant for the salt and pH of this solution. Given ionisation constant of acetic acid is 1.8×10^{-5}.

(3.75, 5, 5, 5)

Unique Paper Code	: 32171101
Name of the Paper	:C1: Inorganic Chemistry –I (Atomic Structure and Chemical Bonding)
Name of the Course	: B.Sc. (H) Chemistry
Semester	: I
Duration	: 3 Hours
Maximum Marks	: 75

Instructions for Candidates

(i) Attempt any **four** questions.
(ii) A**ll** questions carry equal marks.

1. Explain the following:

(i) The bond angles in the fluoride of nitrogen are less than that of its hydride whereas reverse is true for phosphorous:
$NF_3 = 102.1^o$ $PF_3 = 98^o$
$NH_3 = 107.3^o$ $PH_3 = 94^o$

(ii) Though electron gain enthalpy of chlorine is higher than that of fluorine, yet fluorine is a stronger oxidizing agent than chlorine.

(iii) NaCl is soluble in water but insoluble in CCl_4.

(iv) $CdCO_3$ decomposes at 350º C while $CaCO_3$ at 900º C.

(v) PF_5 exists but PH_5 does not. (5 X 3.5)

2.

(i) Name the three quantum numbers which are obtained by solving the wave equation. What is the significance of each one? State the values which can be assigned to each of these.

(ii) Given the equation: $U_0 = \frac{ANZ^+Z^-e^2}{4\pi\epsilon_0 r_0}\left(1 - \frac{1}{n}\right)$

(a) Name the above equation.
(b) Explain the terms involved.
(c) 'The above equation is self-compensating and tends to hide errors.' Explain this statement.

(iii) Using Band theory explain, explain the electrical conductivity in Be metal.

(iv) Calculate S and Z_{eff} for 3d electron in Cu (Z = 29).

(v) What is meant by well behaved wave function? (5 X 3.5)

3.

(i) Using VSEPR Theory, predict the shapes of the following species:
PCl_4^+, ClF_3, SF_4, I_3^-

(ii) Calculate the ionic radii of K^+ and Cl^-, if the internuclear distance between these ions is 314 pm.

(iii) Arrange the following in order of increasing acidic character and justify.
Methane, ethylene and acetylene.

(iv) Draw radial probability distribution curves for 4s, 4p and 4d orbitals.

(v) Give the mathematical expressions for the condition of normalization and orthogonality. (5 X 3.5)

4.

(i) what are equivalent and non- equivalent hybrid orbitals. Explain with suitable examples.

(ii) Give major difference between orbit and orbital.

(iii) The dipole moment of HI is 0.384D and bond distance is 1.60 pm. What will be the percent of ionic character in HI?

(iv) Arrange the following in order of increasing bond angle and justify.
H_2O, Cl_2O and F_2O.

(v) CO and N_2 are isoelectronic. Explain on the basis of molecular orbital theory that CO is a better electron pair donor through carbon. (5 X 3.75)

5.

(i) State Bent's rule. Predict whether H-C-H angle in CH_2F_2 is higher or lower than tetrahedral angle.

(ii) K^+ and F^- ions have the same size but their considerable difference in the values of their hydration energy. Explain.

(iii) Give reasons why
(a) $PbCl_4$ is more covalent than $PbCl_2$?
(b) Half filled and fully filled orbitals are associated with extra stability?

(iv) Construct the Born Haber cycle and calculate the lattice energy for an ionic salt MO using the following data:
Sublimation enthalpy of M = 178 kJ/mol
First ionization enthalpy of M = 590 kJ/mol
Second ionization enthalpy of M = 1150 kJ/mol
Dissociation enthalpy of O_2 = 498 kJ/mol
First electron affinity of O = -141 kJ/mol
Second electron affinity of O = 798 kJ/mol
Enthalpy of formation = -635 kJ/mol

(v) What type of chemical forces are there when-?
(a) NaCl is added in water?
(b) NH_3 is added in water? (5 X 3.75)

6.

(i) Explain on the basis of Molecular orbital theory which of the following species have identical bond orders:
O_2^-, NO^+ and N_2.
Explain their magnetic behavior also.

(ii) Explain the defects present in non-stoichiometric compounds.

(iii) Write a short note on – Limitations of Aufbau principle.

(iv) In a H- atom, an electron jumps from a third orbit to the first orbit. Give the expression for frequency and wavelength of the spectral line.

(v) $MgSO_4.7H_2O$ is soluble in water whereas $BaSO_4$ is insoluble.

(5 X 3.75)

Unique Paper Code : 32171301

Name of the Paper : Inorganic Chemistry II: s- and p- Block Elements

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

Semester : III

Duration : 3 Hours

Maximum Marks : 75

Instructions for Candidates

- Attempt any ***four*** questions.
- All questions carry equal marks

1. (a) Give reason for the following:
   (i) Arrange the following in order of their increasing Lewis acid strength:
   BBr_3, BCl_3, BF_3
   (ii) As rubidium is added in liquid ammonia gradually, a blue coloured solution is obtained initially, but with more addition of rubidium, a bronze colored layer is formed, which floats on blue colored solution. (3x2)

   (b) (i) Give the principle and procedure of Mond's Process.
   (ii) Using Ellingham diagram, explain why the slope of most of the lines move in upward direction with increase in temperature. (3x2)

   (c) Why is white phosphorus more reactive than red phosphorus? Draw the structure of P_4O_{10} and give the stepwise mechanism of its hydrolysis. (2,1,3.75)

2. (a) (i) Which is more basic? KOH or $Ca(OH)_2$. Why?
   (ii) Arrange the following hydrides in increasing order of their boiling points. Give reason for the same.
   H_2Se, H_2O, H_2Te, H_2S (3x2)

   (b) (i) Oxygen is a gas and exists as O_2, while sulphur is a solid and exists as S_8. Why?
   (ii) Which one will have higher negative electron gain enthalpy: Fluorine or chlorine? Give reason. (3x2)

   (c) (i) On burning Li in air, two compounds **(A)** and **(B)** are obtained. When treated with water, **(A)** liberates NH_3 gas, while aqueous solution of **(B)** is basic in nature. Identify **(A)** and **(B)** and give the balanced chemical reaction(s) involved.
   (ii) What is crown ether? Draw the structure of dibenzo-18-crown-6. (4,2.75)

3. (a) (i) Give the chemical reaction involved on heating: (A) Lithium nitrate, (B) Potassium nitrate and explain the same.
   (ii) Though HF is more ionic than HCl, but it is a weaker acid than HCl in aqueous solution. Why? (3x2)

   (b) (i) Silanes are more reactive than alkanes. Why? Explain your answer with a suitable

example.

(ii) Which will have greater complex forming tendency**:** Rubidium or Strontium? Why? (3x2)

(c) What are interhalogen compounds? How are they different from halogens? Discuss the structures of I_2Cl_6 and BrF_5. (1.75,1,4)

4. (a) Explain the following:

(i) PCl_5 is a Lewis acid while PCl_3 is a Lewis base.

(ii) Alkali metals impart characteristic colour in the Bunsen flame. (3x2)

(b) (i) Give the balanced chemical reactions of the following metals, when heated initially with Carbon, followed by hydrolysis of the products formed:
(A) Beryllium (B) Calcium

(ii) Compare the structures of dimeric beryllium chloride and diborane with respect to bridging bonds present in them. (3x2)

(c) Which type of metals can be purified by Zone refining process. Explain its principle and procedure with diagram. (6.75)

5. (a) (i) Large number of silicates and polyphosphates are known, lesser number of polysulphates are known, but no polychlorates are known. Explain.

(ii) Why IF_7 is not stored in glass bottles? Explain with the help of chemical reaction. (3x2)

(b) Complete the following equations:

(i) $H_2S_2O_8 + H_2O \rightarrow$

(ii) $Cl_2O + NaOH \rightarrow$

(iii) $PCl_3 + H_2O \rightarrow$

(iv) $BrF_5 + H_2O \rightarrow$

(v) $B_2H_6 + O_2 \rightarrow$

(vi) $XeF_6 + NaOH \rightarrow$ (1x6)

(c) Name the different oxoacids of Chlorine. Draw their structures and arrange them in increasing order of their acid strength, giving reason(s). (6.75)

6. (a) Describe the chief modes of occurrence of metals based on standard electrode potentials. (6)

(b) Explain the following:

(i) Which has a greater bond angle? NH_3 or PH_3

(ii) $SO_2(g)$ and $SO_3(g)$ have the same hybridization but different structures. (3x2)

(c) What are silicates? Briefly discuss the different types of silicates. Give their structures and uses. (6.75)

SET A

Sr. No. of Question Paper :

Unique Paper Code : 32173911

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

Name of the Paper : Pesticide Chemistry: Skill Enhancement Course

Semester : III

Duration : 3 Hours Maximum Marks: 38

Instructions for Candidates

1. Write your roll number, Name of the Paper, Course, Semester, and Date of examination on the first page of the answer sheet.
2. Attempt **ANY FOUR** questions. All questions carry equal marks.

1. State the classification of pesticides on the basis of their chemical nature, use and chemical structure. Name and draw different isomers of DDT with their decreasing order of toxicity. (9.5)

2. "Botanical insecticides are like alternatives of conventional pesticides." Comment on the statement. Give at least five examples of botanical insecticides with their structures and uses. (9.5)

3. What are controlled release formulations? How they work? How these formulations are better than Wettable powders, dust and Emulsifiable concentrates? (9.5)

4. Explain role of integrated pest management in the pest control strategy. Name and explain at least four biological pest control tools. (9.5)

5. (1) "Organophosphates are known as nerve agents". Explain their interaction with nervous system.
   (2) Discuss the mode of action and synthesis of Carbamate. (4.5, 5)

6. Discuss structure activity relationship (SAR) to design a particular pesticide with reference to its physical and biological property. (9.5)

SET: 2

Unique Paper Code: 32171301-OC

Name of the Paper: Inorganic Chemistry-II; s and p block elements.

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

Semester: III

Duration: 3 Hours

Maximum Marks: 75

Instructions for Candidates:

1. Attempt any **four** questions.
2. All questions carry equal marks.

1. (a) Discuss the anomalous behavior of Lithium and its compounds with respect to the other alkali metals. (5)

   (b) Explain the following:

   (i) BF_3 exists but BH_3 does not. Why does BH_3 exist as B_2H_6? (2.5)

   (ii) H_3PO_3 is a dibasic acid and is less acidic than H_3PO_4 (2.5)

   (c) Describe different types of interhalogen compounds. Why are inter-halogen compounds more reactive than halogens? (5)

   (d) What is Cairo's acid, give its structure. (3.75)

2. (a) Name various oxy acids of chlorine and discuss their relative strength. (5)

   (b) Solutions of alkali metals in liquid ammonia show different properties as the metal concentration increases. Explain. (5)

(c) Draw the structure of $BeCl_2$ in vapour phase and solid phase. What is the oxidation state of Be in each case? (5)

(d) What is Vapour Phase Refining? Discuss any one method. (3.75)

3. (a) Name the class of silicates for the following minerals: (5)

(i) Mica (ii) Benitoite (iii) Asbestos (iv) Zircon (v) Ultramarines

(b) Draw structures of the following molecules giving the hybridization of the central atom. (5)

(i) B_2H_6 (ii) PCl_5

(c) What happens when: (5)

B_2H_6 + excess NH3 $\rightarrow$

Cl_2O_6 + NaOH $\rightarrow$

$AlCl_3$ + $NaBH_4$ $\rightarrow$

HN_3 + HNO_2 $\rightarrow$

P_2O_5 + NaOH $\rightarrow$

(d) Which is more ionic: PbO or PbO_2? Explain. (3.75)

4. (a) Carbon can be a good reducing agent over a wide range of temperature, explain with Ellingham diagram. (5)

(b) Discuss unique characteristics of crown ethers and cryptates as ligands. (5)

(c) How are Phosphazenes prepared? Give their three impotent properties. (5)

(d) Phosphoric acid is syrupy and viscous. Comment. (3.75)

5. (a) What is diagonal relationship? B and Si show similar behavior, explain with examples. (5)

(b) Describe different allotropes of Phosphorus. (5)

(c) What are clathrates compounds? Discuss with respect to noble gas clathrates. (5)

(d) Pseudo halogens resemble halogens. Discuss. (3.75)

6. (a) What are Silicones? How are silicones prepared? Why are they chemically important? (5)

(b) What is inorganic benzene? Why is it so called? Explain its higher reactivity as compared to that of benzene. (5)

(c) Explain

(i) Which is more stable $SnCl_2$ or $SnCl_4$? (2.5)

(ii) Effect of heat on Sulphur. (2.5)

(d) Magnesium does not impart any colour to the flame while calcium does, why? (3.75)

R.Rastogi

Roll No……

S. No. of Question Paper :

Unique Paper Code : **32173909**

Name of the Paper : **Pharmaceutical Chemistry**

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

Semester : III

Duration: 1.5 Hours Maximum Marks: 38

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **four** questions.
3. Each question carries 9.5 marks.

1. (i) Describe the Drug Discovery and Development procedure. (4)
   (ii) What are analgesics? How do these drugs affect our body? Give an example. (4)
   (iii) Difference between antibiotics and antibacterial agents. (1.5)

2. (i) Write short note on any one of the following: (4)
   (a) Antifungal drugs
   (b) Pharmaceutical aids
   (ii) Describe the fermentation procedure for synthesis of streptomycin. (4)
   (iii) Difference between side effects and toxicology effects of medicine. (1.5)

3. (i) What are central nervous system agents? Give two examples with structure. (4)
   (ii) Define following terms with suitable examples: (2 x 2 = 4)
   (a) Antipyretic agents
   (b) Antilaprosyl drugs
   (iii) Distinguish between bacteriostatic and bactericidal agents. (1.5)

4. (i) Mention the side effects of thalidomide and ibuprofen. (4)

(ii) What are anti-inflammatory agents? How do they work? Give an example. (4)

(iii) Differentiate between drugs and poisons. (1.5)

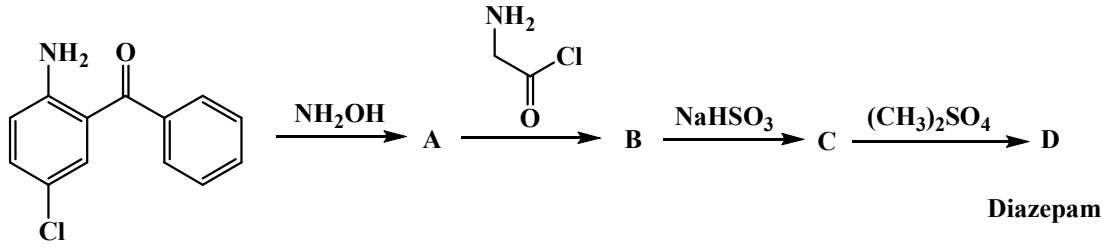
5. (i) What is drug-receptor interaction? Explain with illustration. (4)

(ii) Match the following: (1 x 4 = 4)

Column A	Column B
Saccharomyces cerevisiae	Cephalosporin
Antiviral agent	Glyceryl nitrate
Cardiovascular drug	Ethanol
Acremonium chrysogenum	Acyclovir

(iii) Write the chemical reaction for synthesis of glyceryl trinitrate. (1.5)

6. (i) Mention the structure of the compounds A-D. (4)



Diazepam

(ii) Describe the fermentation synthesis procedure of vitamin C. (4)

(iii) Draw the chemical structure of cephalosporin and streptomycin. (1.5)

Unique Paper Code	**:**	32171302_OC
Name of the Paper	**:**	Chemistry C-VI Organic Chemistry-II Oxygen Containing Functional Groups
Semester	**:**	III
Name of the Course	**:**	B.Sc. (H) Chemistry
Duration	**:**	3 hours
Maximum Marks	**:**	75

Instructions for Candidates:

(i) Attempt four questions in all. Question No. 1 is compulsory.
(ii) Give reactions wherever possible clearly indicating the reagent(s) involved.

1. **(12,6,3)**

(a) An organic compound **A** ($C_6H_{12}O_2$) on reduction with $LiAlH_4$, yielded two compound **B** and **C**. Compound **B** on oxidation gave compound **D**, which on treatment with aqueous alkali and subsequent heating furnished compound **E**. The latter on catalytic hydrogenation gave compound **C**. The compound **D** was oxidized to give compound **F**, which was found to be a monobasic acid (molecular formula wt. = 60 g). Deduce the structure of compounds **A**-**F**, write the reactions involved and give the mechanism of formation of compound **E** from compound **D**. Also give the name of the reaction involved.

(b) How you will distinguish the following, Give visible test:

(i) Chlorobenzene and Chloroethane

(ii) Propnaldehyde and Benzaldehyde

(iii) Phenol and *p*-Cresol

(c) What happens when Benzamide is heated with Bromine and sodium hydroxide. Write the product, mechanism, and name of the reaction involved

2. **(9,9)**

(a) How will you prepare the following using ethyl acetoacetate synthesis:

(i) 3-Methylpentan-2-one

(ii) Pentane-1,5-dioic acid

(iii) *n*-Butyric acid

(b) How will you prepare the following using Diethyl malonate synthesis:

(i) 2-Methyl hexanoic acid

(ii) Succinic acid

(iii) 5,5-Diethyl barbituric acid

3. **(12,6)**

(a) Explain the following:

(i) '-R' group at ortho and para position facilitates aryl halides towards Aromatic Nucleophillic Substitution Reaction

(ii) The role of pH during the reaction of carbonyl compounds with ammonia and its derivatives.

(iii) Enol form of ethylacetoacetate is more stable than that of ethyl acetate.

(iv) The rate of hydrolysis of carboxylic acid derivatives is:

$CH_3COCl > (CH_3CO)_2O > CH_3CONH_2$

(b) How will you carry out the following conversions (Attempt any *two*):

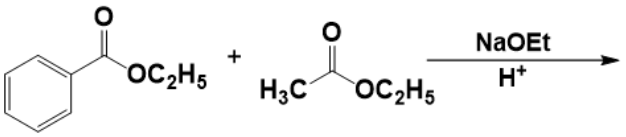
(i) Phenol to Asprin

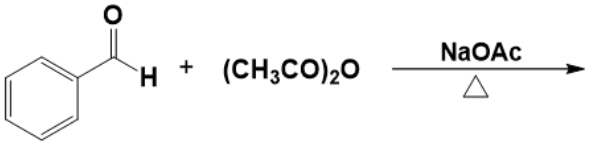
(ii) Propanal to 2-butanol

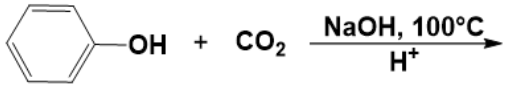
(iii) Propanoic acid to lactic acid

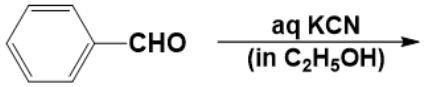
4. **(4 x 4.5 = 18)**

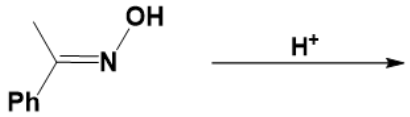
(a) Complete the following reactions. Give the name of the reaction along with the mechanism (Attempt any *four*):

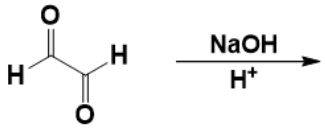
(i) 

(ii) 

(iii) 

(iv) 

(v) 

(vi) 

5. **(15, 3)**

(a) What happens when:

(i) Alpha, beta, and gamma hydroxy acids are heated separately.

(ii) Glycerol is treated with periodic acid.

(iii) Chloro benzene is heated with Soda amide.

(iv) 2,3-Dimethyl butan-2,3-diol is treated with H_2SO_4.

(v) Ethylene oxide when treated with Phenyl Magnesium Bromide followed by acidification.

(b) Prepare the following:

(i) Phenetole

(ii) Methyl *tert*-butyl ether

6. Write a short note on any ***three*** of the followings: (**6x3 = 18**)

(a) Michael Addition

(b) Fries Rearrangement

(c) Baeyer-Villiger Oxidation

(d) Keto-enol Tautomerization

(e) Reformatsky Reaction

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Roll No……..

S. No. of Question Paper	:	
Unique Paper Code	:	**32173909**
Name of the Paper	:	**Pharmaceutical Chemistry**
Name of the Course	:	**B.Sc. (H) Chemistry**
Semester	:	III

Duration: 3 Hours Maximum Marks: 38

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **four** questions.
3. Each question carries 9.5 marks.

1. (i) Describe the laboratory synthesis of paracetamol and its mode of action. (4)
   (ii) Discuss the production of ethyl alcohol through anaerobic fermentation. (4)
   (iii) Differentiate between narrow-spectrum and broad-spectrum antibiotics. (1.5)

2. (i) Explain retrosynthetic approach in drug discovery. Write down retrosynthetic pathway of paracetamol. (4)
   (ii) What is the role of gelatin and kaolin as pharmaceutical aids in drug formulation? (4)
   (iii) What is the meaning of 'High Therapeutic Index'? (1.5)

3. (i) Write short note on any one of the followings: (4)
   (a) Lead Compound
   (b) Bioisosteres
   (ii) What are drugs and what is the role of SAR studies in drug development? (4)
   (iii) What are the side effects of cetirizine and thalidomide? (1.5)

4. (i) Describe the fermentation process for production of glutamic acid. (4)
   (ii) Define following terms with suitable examples: (2 x 2 = 4)
   (a) Antiviral agents
   (b) Cardiovascular drugs

(iii) Define the term 'Synergism'. (1.5)

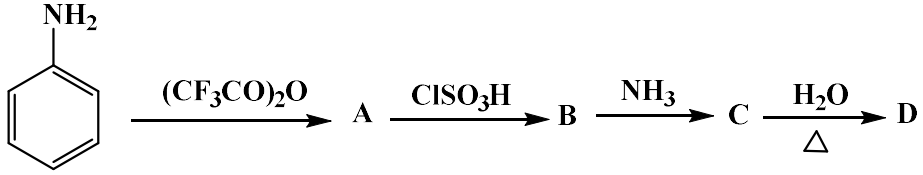
5. (i) Write down the chemical synthesis of sulfamethoxazole with its therapeutic uses and adverse effects. (4)

(ii) Match the following: (1 x 4 = 4)

Column A	Column B
Ascorbic Acid	Vitamin B_{12}
Cobalt	Streptomycin
Aspergillus niger	Vitamin C
Streptomycin griseus	Citric Acid

(iii) Write the full name of 7-ACA and draw its chemical structure. (1.5)

6. (i) Mention the structure of the compounds A-D. (4)



Sulphanilamide

(ii) How can Penicillin be produced commercially using fermentation method? (4)

(iii) Differentiate between 'potency' and 'efficacy' of drugs. (1.5)

Unique Paper Code : 32171303_OC

Name of the Paper : Physical Chemistry III: Phase Equilibria and Electrochemical Cells

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

Semester : **III**

Duration: 3 Hours Maximum Marks: 75

Instructions for Candidate

Attempt four questions in all, selecting at least two questions from each section.

Use of scientific calculator is permitted

Values of constant: R = 8.314 JK^{-1} Mol^{-1}; F = 96500 C Mol^{-1}

Section-A

Q.1.a) Derive the Clapeyron equation and then derive Clausius-Clapeyron equation for condensed phase-vapour system. Does this relation hold good for the solid to liquid equillibria? Justify your answer.

b) Calculate the number of components in a solution containing H^+, OH^-, Na^+, Cl^-, Ag^+, NO_3^-, AgCl (s) & H_2O (l). Show all the constituents, reactions & restrictive conditions.

c) An aqueous solution contains 0.30 g of a solute in 100 cm^3 solution. To this solution 25 cm^3 of ether is added and the mixture is shaken and allowed to come to equilibrium at 298K. At this temperature, $K_d = C_{ether}/C_{water} = 4.7$

i) How much solute remains in the aqueous solution?

ii) If the extraction is carried out with two successive 20 cm^3 portions of ether, how much solute remains unextracted?

d) What is Gibbs Duhem equation? Use this equation for a binary solution to derive Duhem-Margules equation.

(5, 5,5,3.75)

Q.2. a) Differentiate between congruent & incongruent melting point systems with an example for each. Why both of them are invariant points?

b) Describe the phase diagram of water with due emphasis on following facts:

i) How many triple points does it have?

ii) Why is sublimation curve steeper than the vaporization curve at triple point?

iii) Why is fusion line almost vertical & slightly tilted to the left?

iv) What is the upper limit of liquid-vapour equilibrium curve?

c) Describe the process of fractional distillation of an ideal binary solution with the help of suitable diagrams along with the principle underlying it.

d) What are azeotropes? Give one example each of maximum boiling & minimum boiling azeotropes. Can they be purified by fractional distillation?

(5,5,5,3.75)

Q.3. a) Plot a labeled phase diagram (with degrees of freedom) of a system with components: A (M.Pt: 1100 ^{o}C) and B (M.Pt: 600 ^{o}C). The eutectic temperature is 400 ^{o}C and the corresponding composition is 85 mol % of B. Draw the labeled cooling curves for the solutions containing 100 mol% of A, 85 mo% of B & 56 mol% of B.

b) Deduce Gibbs Phase rule for a non-reactive system at equilibrium in which all the components are present in all the phases.

c) State Nernst Distribution Law. Derive the expression for Nernst Distribution Law when the solute undergoes dissociation in one of the phases.

d) Discuss the effect of adding following impurities on CST of phenol-water system:

i) NaCl ii) Succinic Acid

(5,5,5,3.75)

Section-B

Q.4. a) Explain a method to determine the accurate value of half-cell potential graphically.

b) Construct the galvanic cell for the following reaction and write down the expression for the cell potential,

$$\boldsymbol{AgCl(s) + I^{-}(aq) \rightleftharpoons AgI(s) + Cl^{-}(aq)}$$

c) Determine the standard equilibrium constant of the following reaction at 298K

$$\boldsymbol{Cu(OH)_2 \rightleftharpoons Cu^{2+}(aq) + 2OH^{-}(aq)}$$

$$\boldsymbol{Given\ that\ E^{o}_{Cu(OH)_2, OH^{-}/Cu} = -0.224\ V\ and\ E^{o}_{Cu^{2+}/Cu} = 0.337\ V}$$

d) Why is the Mercurous Chloride written as Hg_2Cl_2 not as HgCl?

(5,5,5,3.75)

Q.5. a) Derive the expression for the EMF of a concentration cell with transference.

b) Write the BET equation and derive the Langmuir adsorption isotherm from it.

c) Determine the cell potential for the following cell at 25°C assuming the activity equal to molar concentration

$$Mg|MgI_2\ (0.1\ mol\ dm^{-3}|I_2|Pt$$

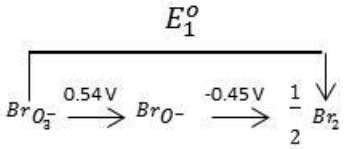
$$\boldsymbol{Given\ that\ E^o_{I^-/I_2/Pt} = -0.535\ V\ and\ E^o_{Mg^{2+}/Mg} = -2.363\ V}$$

d) Can a voltmeter be used to determine the EMF of a galvanic cell?

(5,5,5,3.75)

Q.6.a) Describe the construction of calomel electrode. Write the half-cell reaction and Nernst equation for it.

b) From the standard potentials shown in the following diagram, calculate the potential(E_1^o)



c) Write a short note on potentiometric titrations

d) What are the limitations of Quinhydrone electrode for the determination of pH of solution?

(5,5,5,3.75)

SET – A

Name of Course : B Sc (Hons.) Chemistry

Semester : III

Name of the Paper : Organic Chemistry II(Halogenated hydrocarbons and Oxygen Containing Functional Groups)

Unique Paper Code : 32171302

Duration : 3 hrs

Maximum Marks :75

Instructions for candidates

1. Attempt any 4 questions
2. Attempt all parts of a question at one place
3. All questions carry equal marks

1.

a) What happens when benzaldehyde is treated with (Explain with mechanism)
   i. Aqueous alcoholic KCN
   ii. Hydrazine

b) A ketone (A) gives iodoform test. (A) on hydrogenation gives (B) which on heating with H_2SO_4 gives (C). Action of O_3 on (C) gives (D) which when treated with water in presence of Zn dust gives only acetaldehyde. Identify (A), (B), (C), (D) and write the reactions involved.

c) Explain the following
   i. Acid catalyses the addition of semi-carbazide to acetone, but too much acidity of medium is harmful for the reaction.
   ii. Why acetaldehyde is more reactive than acetone towards nucleophilic addition?

d) Synthesize the following using diethyl malonate
   i. Barbituric acid
   ii. 3-methyl butanoic acid

e) Mention a reagent to which acetaldehyde and benzaldehyde react similarly and another reagent to which they react differently also write the reactions.

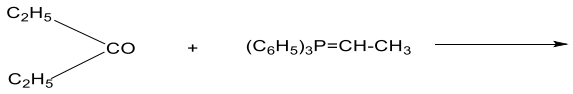
(4,4,4,4,2.75)

2.

a) How will you obtain the following from acetoacetic ester (any 2)
   i. Isobutyric acid
   ii. Methyl propyl ketone
   iii. Acetyl acetone

b) benzaldehyde $\xrightarrow{CH3MgI\ /\ H3O}$ A $\xrightarrow{mild\ oxd.}$ B $\xrightarrow{I2/OH-}$ C
Identify A, B, C

c) Complete and name following reaction
   i. $(CH_3)_3CCHO + (CH_3)_3CCHO \xrightarrow{50\%\ NaOH}$

ii. 

iii. $C_6H_5CHO + (C_6H_5)_3P{=}CH_2 \longrightarrow$

iv. $C_5H_5CHO + CH_2(COOC_2H_5)_2 \longrightarrow$

d) Explain the following
   i. How you can differentiate between acetaldehyde and acetone. Write the reaction also
   ii. How you can differentiate between acetaldehyde and benzaldehyde. Write the reaction also

e) How you can convert butanone to
   i. 2-butanol
   ii. n-butane

(4,4,4,4,2.75)

3. Explain
   i. Neopentyl halide are notoriously slow in nucleophilic substitution whatever the experimental conditions are
   ii. Which of the following 2 synthesis is preferred for tertiary butyl ether
      1. $(CH_3)_3CO^- + CH_3CH_2Br \longrightarrow$
      2. $(CH_3)_3C\text{-}Br + CH_3CH_2O^- \longrightarrow$

   b) Compare the reactivity of chlorobenzene and 2,4 – dinitrochlorobenzene towards NaOH
   c) Account for the formation of m-$MeOC_6H_4NH_2$ from ammonolysis of either o- $MeOC_6H_4Br$ and m-$MeOC_6H_4Br$
   d) Give the major product and mechanism for the following reactions
      i. $CH_3CH_2CH_2CH_2Br + CH_3O^- + CH_3OH^- \longrightarrow$
      ii. $(CH_3)_3CBr + {}^-SH + C_2H_5OH \xrightarrow{50°C}$
   e) Nitration of bromobenzene is much faster than bromination of nitrobenzene

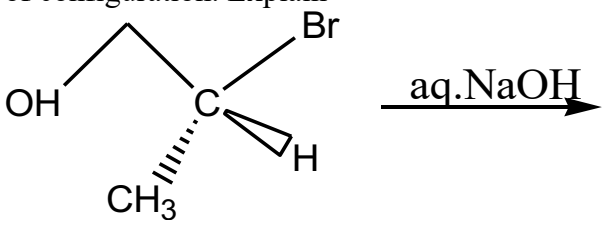
(4,4,4,4,2.75)

4.
   a) Acid or base catalyzed hydrolysis of $(C_2H_5)_3C - CN$ proceeds up to amide stage. The corresponding acid is not obtained
   b) Give the mechanism of hydrolysis of methyl benzoate by $NaOCH_3$ in CH_3OH.
   c) How can an ester be converted to beta keto ester what is the name of the reaction? Explain with mechanism
   d) Give the mechanism of ethanamide with bromine in presence of KOH
   e) Giving reasons arrange the following acids in increasing order of acidity CH_2Cl-COOH, CH_3- COOH, $CH_2{=}CHCH_2COOH$, CI_3COOH

(4,4,4,4,2.75)

5.
   a) Write the structure of alcohol formed from $(CH_3)_2C{=}CH\text{-}CH_3$ on hydroboration - oxidation, give the mechanism involved.
   b) How will you carry out the following conversions
      i. Acetone to 2-methyl-2-butanol
      ii. n-propanol to butanamide
   c) Write a test along with reaction involved to distinguish between the following pairs of compounds
      i. Phenol and Benzyl alcohol
      ii. Ethyl alcohol and Diethyl ether

d) Why the substitution of bromine in the following reaction proceeds with retention of configuration. Explain

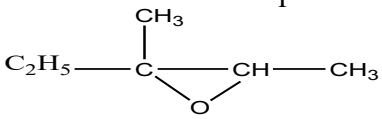


e) What products are formed when Anisole is heated with HI? Explain with the help of mechanism.

(4,4,4,4,2.75)

6.

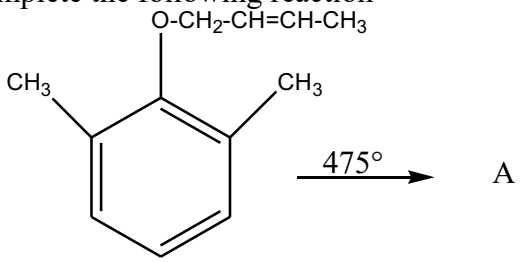
a) Write the reaction sequence involved in the ring opening



with methanol in presence of acid.Explain the formation of different products on reaction with sodium methoxide.

b) Compare the solubility,volatility and acidity of o-nitrophenol and p-nitrophenol.

c) Complete the following reaction



Identify A, name of the reaction and explain the formation of A with mechanism.

d) Explain the order of reactivity of the following compounds with HBr and mechanism involved Ph_2CHOH, $PhCH_2OH$, p-NO_2-Ph-CH_2OH, p-Cl-Ph-CH_2OH

e) In the following reaction Name the reagent and identify A.

$(CH_3)_2C(OH)CH_3$. $\xrightarrow{Fe2+,H2O2}$

(4,4,4,4,2.75)

SET A

[This question paper contains 2 printed pages]

Sr. No. of Question paper Roll No……

Unique Paper Code : 32171501_OC

Name of the Paper : Organic Chemistry IV: Biomolecules

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

Semester : V

Duration : 3 Hours

Maximum Marks : 75 Marks

Instructions for Candidate

1. Attempt the paper on plain white sheets only.
2. Each sheet is to be numbered and signed at the top.
3. Answer four questions in all. All questions carry equal marks.

Q.1 (a) What are fat, oil and waxes? Give the structure, numbering and name of an omega-3 fatty acid. Discuss their importance in our diet.

(b) What are saponification value and iodine number? Calculate the iodine number for the glyceryl-trioleate having molecular weight 884.

(c) Explain the hydrogenation and hydrogenolysis of lipids. Write down its application.

(6.25, 6.25, 6.25)

Q.2 (a) Synthesize valanylaspartnylglycine by Merrifield solid phase synthesis. Discuss advantages of solid phase synthesis.

(b) Define isoelectric point and how it can be determined. Draw the pH curve of glutamic acid and calculate the isoelectric point from the following data pka1=2.19, pka2= 4.25 and pka3 = 9.67

(c) Explain one method with reaction to determine C-terminal and N-terminal amino acid of proteins.

(6.25, 6.25, 6.25)

Q.3 (a) Why an electrophilic attack on pyrimidine ring takes place at position 5 of the ring? Explain. Give one synthesis of Thymine.

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

(c) Explain synthesis of Adenine and Guanine by Traube's method.

(6.25, 6.25, 6.25)

Q. 4 (a) What is K_M value? Explain its significance. Explain why there is no increase in the rate of catalysis, with increase in substrate concentration, at high concentration of the substrate in an enzyme catalysed reaction.

(b) Define holoenzyme, apoenzyme, co-enzyme and co-factor with example.

(c) What is enzyme inhibition? Explain the type of enzyme inhibition.

(6.25, 6.25, 6.25)

Q. 5 (a) Give the structure of ATP. Discuss how enzymatic hydrolysis reactions are energy producing reactions.

(b) Define calorific vale of food. Why fats have more calorific value than carbohydrates?

(c) Explain the interrelationship in the metabolic pathway of carbohydrate, fats and proteins.

(6.25, 6.25, 6.25)

Q. 6 (a) Give the structure and IUPAC name of Ibuprofen and write its conventional synthesis.

(b) What are anti-inflammatory agents? Describe synthetic pathway for Ibuprofen.

(c) Write medicinal importance of curcumin and azadirachtin.

(6.25, 6.25, 6.25)

Unique Paper Code : 32171501

Name of Paper : Organic Chemistry IV: Biomolecules

Name of the course : B.Sc. (Hons.)

Semester : V

Duration : 3 hours

Maximum Marks : 75 Marks

Instructions for Candidates

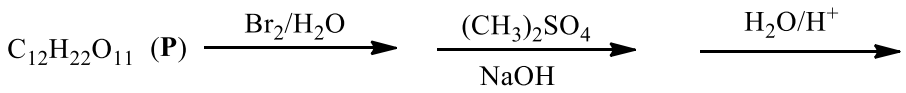
1. *Attempt the paper on plain white sheets only.*

2. *Each sheet is to be numbered and signed at the top.*

3. *Attempt **four** questions in all.*

4. *All questions carry equal marks.*

Q.1 (a) A carbohydrate (**P)** having the molecular formula ($C_{12}H_{22}O_{11}$) is hydrolyzed with *emulsin*, only D-glucose is obtained. **P** reacts with Br_2 water as well as Benedict reagent. Also, when **P** is subjected to following sequence of reactions, **Q** and **R** are produced. Deduce the structure of **P** and also explain the reactions.



2,3,4,6-tetra-*O*-methyl-D-glucose (**Q**) + 2,3,5,6-tetra-*O*-methyl-D-gluconic acid (**R**)

(b) Which form of alanine would you expect to predominate in (i) strongly acidic solution (ii) strongly basic solution and (iii) at its isoelectric point. Indicate which part of the dipolar ion behaves as a potential acid or potential base and also find out the isoelectric point of alanine (pKa_1 = 2.3, pKa_2 = 9.7).

(c) (i) What is the difference between nucleosides and nucleotides? Give the structure of guanosine-5'-triphosphate.

(ii) Give one example of each, ω-3 and ω-6 fatty acids with their structures.

(6.75, 6, 6)

Q.2 (a) Write the Merrifield synthesis of the dipeptide Gly-Val. What are the advantages of this method over other methods?

(b) Rate of glucose mutarotation is slow in D_2O than in H_2O. Explain with mechanism.

(c) How many types of RNA are known which works collectively for the protein synthesis? Explain their roles in brief.

(6.75, 6, 6)

Q.3 (a) What is fermentation? Write down the fate of pyruvate in alcoholic and lactate fermentation with enzymes involved.

(b) Define saponification value and give its significance. Calculate the saponification value of glyceryl tripalmitate having Mol. Wt. 806 (Mol. Wt. of KOH = 56).

(c) Explain the process of Replication of DNA.

(6.75, 6, 6)

Q.4 (a) (i) Write down the role and importance of enzyme *phosphofructokinase* in glycolysis. (ii) Give the structure of NAD^+.

(b) Give the synthesis of Proline by phthalimide malonic ester method.

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

(6.75, 6, 6)

Q.5 (a) What is enzyme inhibition? Explain allosteric inhibition.

(b) 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

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

(6.75, 6, 6)

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

(a) Genetic Code
(b) Starch and Cellulose
(c) Reversion and Rancidity
(d) Secondary Structure of Proteins

(6.25, 6.25, 6.25)

Unique Paper code : 32171502 (OC)

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

Name of the paper : Chemistry C-XII Physical Chemistry V: Quantum Chemistry and Spectroscopy

Semester : V

Duration : 3 hours

Maximum Marks : 75

Instructions for Candidate:

1. **Attempt any FOUR questions in all.**
2. **Each question carries 18.75 marks.**
3. **Preferably attempt all parts of a question together.**
4. **Please show all calculations as each step carries marks.**

Physical constants

Atomic mass unit	:	1.66×10^{-27} kg
Planck's constant	:	6.626×10^{-34} J s
Velocity of Light	:	3×10^{8} m s^{-1}
Boltzmann constant	:	1.381×10^{-23} J K^{-1}
Mass of Electron	:	9.1×10^{-31} kg
Avogadro's number	:	6.023×10^{23} mol^{-1}
Nuclear magneton	:	5.047×10^{-27} J T^{-1}
Bohr magneton	:	9.274×10^{-24} J T^{-1}

1.

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

(i) cos x $(0, 2\pi)$, (ii) $e^{-x}(-\infty, \infty)$, (iii) e^{-x} $(0, \infty)$ (iv) $\sin^{-1} x$ (-1,1)

(b) What are Hermitian operators? Give two examples. Show that the eigenvalues of a Hermitian operator are always real.

(c) Show that the Morse potential:

$$V = D[1 - \exp\{a(r_{eq} - r)\}]^2$$

is reducible to harmonic potential for the lower vibrational levels. Also show that the force constant is given as $k = 2Da^2$

(6, 6, 6.75)

2.

(a) A particle of mass m existing in a one-dimensional box of length a can be represented by the function, $\psi_n = \sin\frac{n\pi x}{a}$. Determine whether it is an eigen function of (i) $\widehat{p_x}$ (ii) $\widehat{p_x^2}$. Give the eigen values if applicable.

(b) A particle of mass m exists in a two-dimensional rectangular box with sides l_x and l_y equal to a and $2a$, respectively. Write the mathematical expression for the energy level E_{n_x,n_y} when the quantum numbers $n_x = n_y = 2$. Suggest values of another set of quantum numbers n_x and n_y for a state which is degenerate with $E_{2,2}$.

(c) What is the essential condition for a molecule to show Raman spectrum? A molecule AB_2 has the following infra-red and Raman spectra:

Wave number (cm^{-1})	Infrared	Raman
589	Active (PQR)	Inactive
1285	Active (PR)	Active (polarized)
2224	Active (PR)	Active (depolarized)

Giving proper explanation arrive at the geometry of the molecule. Assign the wavenumbers to specific vibrations.

(6, 6, 6.75)

3.

(a) The normalized $1s$ atomic orbital for the hydrogen atom is given by the expression :

$$\psi(r) = \frac{1}{\sqrt{\pi a_0^3}}\exp(-r/a_0)$$

where a_0 represents the Bohr radius. Evaluate <r>for the electron in this orbital, given that $\int r^n \exp(-ar)\, dr = \frac{n!}{a^{(n+1)}}$.

(b) Write the trial wave functions and final wave functions of H_2 molecule in the valence bond and molecular orbital treatment. Compare the two functions and discuss their physical significance.

(c) What are overtones and hot bands? A molecule shows a fundamental vibrational frequency corresponding to 2170 cm^{-1}. If the anharmonicity constant is 0.0028, where would the hot band and first overtone appear? What is the effect of increase in temperature on the intensity of hot bands

(6, 6, 6.75)

4.

(a) Plot all the radial probability distribution functions for an electron in hydrogen atom where n =3. Explain the plots briefly.

(b) What is the essential condition for a molecule to be microwave active? The pure microwave spectrum for $^{1}H^{35}Cl$ is observed as a series of lines at 20.7, 41.5, 62.0, 83.0, 103.8 cm^{-1}. Evaluate the rotational constant and the internuclear distance for this molecule.

(c) Set up the Hamiltonian for H_2^+ explaining all the terms. Applying the Born Oppenheimer approximation and write the final expression of Hamiltonian also. Write the LCAO-MO trial wave function of H_2^+. Explain the physical significance of S-overlap integral, J-coulomb integral and K-resonance/exchange integral.

(6, 6, 6.75)

5.

(a) State the variation theorem. Let the particle in a box be represented by the trial function $\psi = x^2 (1 - x)^2$. Applying the variation theorem to the function calculate the ground state energy ($V = 0$ for $0 \leq x \leq l$ and $V = \infty$ elsewhere) and the percentage error. Given the actual $E_o = \frac{h^2}{8ml^2}$ explain whether the trial function satisfies the variation theorem?

(b) Draw the low and high resolution NMR spectrum of CH_3CHO showing the peak corresponding to the reference standard TMS. Briefly explain the spectra drawn indicating the chemical shift, intensity of the peaks and the splitting pattern.

(c) (i) Draw the energy level diagram to explain bonding in the heteronuclear diatomic molecule HF.

(ii) What are the essential criteria for the atomic orbitals to overlap? 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}

(6, 6, 6.75)

6.

(a) What is the essential condition for a molecule to show ESR spectrum. Which of the following will show ESR spectra: **$H^{\cdot}$, CO_2^{-}, CH_3^{+}, NO_2, $C_5H_5^{\cdot}$, Na^{+}.**

(b) Write short notes on the following:

i. Predissociation and dissociation
ii. Configuration interaction
iii. Born – Oppenheimer approximation
iv. Factors affecting the intensity of transition

(2.75, 4x4)

S.No. of question Paper:

Unique Paper code : 32171502

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

Name of the paper : Quantum Chemistry & Spectroscopy

Semester : V

Duration : 3 hours

Maximum Marks : 75

Instruction for Candidate:

1. **Attempt any FOUR questions in all.**
2. **Each question carries 18.75 marks and has four parts.**
3. **Preferably attempt all parts of a question together.**
4. **Please show all calculations as each step carries marks.**
5. **Use of scientific calculators is allowed.**
6. **This question paper consists of FIVE pages.**

Physical constants

Atomic mass unit	$1.66 \times 10^{-27} kg$
Planck's constant	$6.626 \times 10^{-34} Js$
Velocity of light	$3 \times 10^{8} ms^{-1}$
Boltzmann constant	$1.381 \times 10^{-23} JK^{-1}$
Mass of electron	$9.1 \times 10^{-31} kg$
Avogadro's number	$6.023 \times 10^{23} mol^{-1}$
Nuclear magneton	$5.05 \times 10^{-27} JT^{-1}$
Bohr magneton	$9.274 \times 10^{-24} JT^{-1}$

1. (a) Determine whether the following functions are acceptable or not acceptable as state functions over the interval indicated. Give reasons.

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

(b) Are the following functions eigen functions of the given operators?

Function	Operator
$\left\{sin\left(\frac{3\pi x}{4}\right)\right\}$	$\left(-\frac{h^2}{8m}\frac{d^2}{dx^2} + 0.8\right)$
$\{exp(-x^3/2)\}$	$\left(\frac{d^2}{dx^2}\right)$

If yes calculate the eigen values.

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

(d) Using the quantum mechanical treatment for the hydrogen atom explains the following conclusions:

(i) The energy of relative motion of the hydrogen atom is quantized and this energy is related generally to the distance of electron from the nucleus and does not depend on angular orientation.

(ii) *s* orbitals are spherically symmetrical, but the *p* orbitals are dumbbell shaped.

(5, 5, 5, 3.75)

2. (a) A particle of mass m exists in a one-dimensional box of length a. Using the trial wave function $\psi_{trial} = Ax\left\{1 - \left(\frac{x}{a}\right)\right\}$ 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 the wave functions describing the $1s$ atomic orbital and the $2s$ atomic orbital for the hydrogen atom are orthogonal. Given that:

$\psi_{1s} = (\pi a_0^3)^{-½} \exp(-r/a_0)$ 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 $\int r^n\, exp(-ar)\, dr = n!/a^{(n+1)}$.

(c) Calculate the two possible values of energy for the ^{1}H nucleus placed in an external magnetic field of $5.50T$. What will be the value of ΔE for the splitting observed? Calculate the value of the electromagnetic radiation frequency required to induce a transition corresponding to ΔE. Calculate the relative population of the two states in equilibrium at $300K$. ($g_n = 5.585$)

(d) Prove that if the operators $\hat{A}$ and $\hat{B}$ have the same set of eigen functions then the operators must commute. (5, 5, 5, 3.75)

3. (a) A linear molecule whose moment of inertia is $I = 7.16x10^{-46}kgm^2$ is analysed by a Raman spectrometer using incident radiation at $435nm$. Draw the expected stick-line spectrum under Raman rotational spectroscopy. Where will the first Stokes and Anti-Stokes line appear?

(b) Draw the ψ and ψ^2 patterns for various levels of the Simple Harmonic Oscillator. What conclusions can be drawn from these patterns? How do these compare and contrast with the classical model.

(c) A particle of mass m exists in a cubical box of length a. What is the degeneracy of the state which has energy $\frac{27\,h^2}{8ma^2}$? Write the mathematical expressions corresponding to the degenerate functions to show that they are different eigen functions.

(d) How is it possible to determine the expectation values for a particular observable if the wave function describing the system is not an eigen function of the operator corresponding to the variable? From where does this method originate? Explain with an example. (5, 5, 5, 3.75)

4. (a) The Free Electron Molecular Orbital (FEMO) model has been used to explain bonding and the HOMO to LUMO transitions in the hexa - 1,3,5 – triene molecule. Calculate the wave number corresponding to the $\pi \rightarrow \pi^*$ transition, given that the bond lengths are: C-C : $154pm$; C=C : $135pm$.

(b) Consider the two molecules ^{1}H^{35}Cl and ^{1}H^{37}Cl. Both the molecules are rotating within the rigid rotator approximation and vibrating within the harmonic oscillator model. Their rotational constants are B and B' respectively and their fundamental vibrational frequencies are ν and ν' respectively. Evaluate the ratio of (i) their rotational constants and (ii) their fundamental vibrational frequencies.

(c) The ^1H NMR spectra of CH_3F, CH_3Cl, CH_3Br and CH_3I are run using an instrument operating at $100MHz$. The chemical shifts of the methyl protons are observed at different values on the δ scale. Explain this difference. Will the chemical shift value change if the spectra are run using an instrument operating at $200MHz$? Explain briefly.

(d) For HCl at room temperature three vibrational signals appear at 1198nm, 1764nm and 3465nm. Identify the signals and give the expressions for the energies of transitions corresponding to these. (5, 5, 5, 3.75)

5. (a) The vibrational – rotational spectrum of $^1H^{79}Br$ consists of a series of lines in the P- and R- branches:

P-branch		**R-branch**	
Line	**Position / cm^{-1}**	**Line**	**Position / cm^{-1}**
P_1	2542.56	R_0	2575.55
P_2	2525.51	R_1	2591.23
P_3	2507.86	R_2	2606.61
P_4	2489.63	R_3	2621.35

(i) Draw the spectrum as per data given in the table above.
(ii) What are the values of the rotational quantum numbers J'' and J' for each of the lines observed?
(iii) Evaluate the internuclear distance for the molecule $^1H^{79}Br$
(iv) Evaluate the fundamental vibrational frequency for the molecule.

(b) A particle of mass m exists in a two-dimensional box which extends along both the *x*-axis and *y*-axis. Suppose $\psi(x, y)$ and $\varphi(x, y)$ are two degenerate functions which are solutions to this system. Show that the two possible linear combinations of these two functions are also eigen functions of the system with the same energy.

(c) The time gap between absorption and emission in Phosphorescence is much longer compared to that in case of Fluorescence. In Phosphorescence phenomenon, the absorption spectrum is generally observed at higher wave numbers compared to the emission spectrum. Explain these observations. What kind of information can be obtained from the absorption and emission Phosphorescence spectra?

(d) What is the main difficulty in solving the Schrodinger equation for the Helium atom? Briefly explain the various steps taken to overcome this problem.

(5, 5, 5, 3.75)

6. (a) The vibrational energy levels of $^{23}Na^{127}I$ are:

$$129.3, 389.5, 651.9, 916.5\ cm^{-1}$$

Evaluate the force constant, zero point energy and the bond dissociation energy.

(b) The $J = 2 \rightarrow J = 3$ pure rotational transition for $^{39}K^{37}Cl$ occurs at $22410 MHz$. Assuming that the molecule is rotating under the rigid rotator approximation, predict the frequency and the corresponding wavelength of the $J = 0 \rightarrow J = 1$ transition for both $^{39}K^{37}Cl$ and $^{39}K^{35}Cl$ molecules.

(c) Methanol has a UV absorption peak at $184nm$ with $\varepsilon = 150\ dm^3 mol^{-1} cm^{-1}$. Calculate the transmittance of $184nm$ radiation through a $0.0010\ mol\ dm^{-3}$ solution of methanol in a non-absorbing solvent for two different cells of length: (i) $1.0cm$ and (ii) $10.0cm$.

(d) What is the significance of continuum in the vibrational electronic spectrum of a molecule? In some of the spectra, the continuum is observed in between, followed by discrete lines. What is this phenomenon called and how does it occur?

(5, 5, 5, 3.75)

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

Semester: III

Name of Paper: SEC - Chemistry of Cosmetics and Perfumes

Unique Paper Code: 32173910

Time: 3 Hours **Maximum Marks: 38**

Instructions to Students:

Attempt any **two** questions. All questions carry equal marks.

1.	(a)	What are cosmetics? How are they different from drugs?	3
	(b)	What is the role of boric acid in powder preparations?	2
	(c)	Discuss the mode of action of oxidative hair dyes.	4.5
2.	(a)	Discuss the structure of human hair.	5
	(b)	What are the ideal characteristics of a good hair spray?	3.5
	(c)	Give an example of sequestering agent used in shampoos.	1
3.	(a)	Write a short note on oral hygiene products.	5
	(b)	Discuss the synthesis of a nail paint and nail paint remover.	4.5
4	(a)	Identify the cosmetic product from the ingredients given below, and briefly discuss the role of these in formulation of the given cosmetic product. Stearic acid, potassium hydroxide, glycerin, parabens, lanolin and perfume.	5
	(b)	What are the differences between baby powder and talcum powder?	3
	(c)	What are volatile oils? Give an example.	1.5
5.	(a)	What is SPF? What are the different ingredients used in the synthesis of Sunscreens. Discuss their role.	5

	(b)	What are the ideal characteristics of a good shampoo?	4.5
6.	(a)	Write the structure of muscone and discuss its uses in cosmetic industry.	5
	(b)	Discuss in detail the process of steam distillation used for extraction of sandalwood oil.	4.5

Sl. No. of Q. Paper

Unique Paper Code : 32173910_OC

Name of Paper : SEC- Chemistry of Cosmetics and Perfumes

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

Semester : III/V

Duration : **3 hours** Maximum Marks : **38**

Instructions for Candidates

Attempt all the parts of any **two** questions. All questions carry equal marks.

1. (a) What are the key ingredients involved in the formulation of a lipstick? Also, discuss the method for manufacturing a lipstick.
   (b) Discuss the classification of Hair dyes. Give a detailed account on Oxidative hair dyes.
   (c) Distinguish between the following
      i. Talcum powder and Face powder
      ii. Cold cream and Vanishing Cream
   (d) What is the significance of SPF in a sunscreen lotion? **(5,5,5,4)**
2. (a) Write short notes on any two of the following
      i. Hair spray
      ii. Nail polish
      iii. Hair Conditioners
   (b) What are the various methods for the extraction of essential oils? Explain any one method used for the extraction of 'Rose Absolutes'.
   (c) Discuss the role of various key ingredients used in the preparation of an antidandruff shampoo.
   (d) Explain the role of Borax in the formulation of a Cold Cream. **(5,5,5,4)**
3. (a) Discuss the two main cosmetic products which help in tackling sweat and body odour.
   (b) ‘A cosmetic can mimic a drug'. Justify the statement.
   (c) Discuss the relevance of using preservatives and emulsifying agents in cosmetic products.
   (d) Discuss the mechanism of action of surfactants in a hair shampoo. **(5,5,5,4)**

4. (a) Discuss the structure of skin. Also, write some salient features of an ideal skin preparation.

   (b) What are the characteristics of a good shaving preparation?

   (c) Write any two merits and two demerits of a permanent hair dye.

   (d) What are Artificial flavours? Explain their importance in Cosmetics using examples.

(5,5,5,4)

Unique Paper Code	:	32177903_OC
Name of the Paper	:	DSE- Applications of Computers in Chemistry
Name of the Course	:	B.Sc. (H) Chemistry
Semester	:	V
Duration	:	3 hours
Maximum Marks	:	75

Instructions for Candidates

1. All questions carry equal marks.
2. Answer ***four*** questions in all.
3. Attempt all parts of a question together.

Q1 a) DOS supports only _____ bit programs. **0.75**

b) Write the following algebraic expressions in BASIC.

(i) $\Lambda_m = \Lambda_m^o - k\sqrt{c}$

(ii) $\lambda = \frac{h}{(2meV)^{1/2}}$

(iii) $A = \frac{siny}{log_{10}x}$ **6**

c) The following segment is supposed to check whether the input number lies between 50 and 100. Correct the logic errors so that it can run correctly.

```
10 PRINT "ENTER A NUMBER BETWEEN 50 AND 100"
20 INPUT "NUMBER = "; X
30 IF (X>=50) AND (X>=100) THEN 10
40 PRINT "NUMBER LIES BETWEEN 50 AND 100"
```

6

d) Write a program in BASIC to plot function $f(x)$ in the middle of the monitor screen, for a particle in one dimensional box of length L, for energy level 'n' entered by user in a box.

$$f(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

6

Q2 a) 1TB = _____ GB. **0.75**

b) Differentiate between the following:

(i) Interpreter and Compiler

(ii) Hardware and Software

(iii) Machine Language and Assemble Language **6**

c) Convert the following number systems and show the conversion steps:

(i) $(1011001010)_2$ to Octal Number System

(ii) $(10110110101)_2$ to Hexadecimal Number System

(iii) $(423)_{10}$ to Hexadecimal Number System **6**

d) Explain binary bisection method to find the root of a polynomial. Write a program in BASIC to find pH of weak acid for a 0.1 M concentration of acid at 25°C. Given dissociation constant of acid at 25°C is 1.8×10^{-5} **6**

Q3 a) 'Not equal to' is indicated by _____ in BASIC. **0.75**

b) Explain the role of the following library functions with examples.
(i) INT
(ii) SGN
(iii) MOD **6**

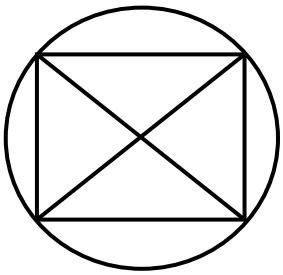
c) Following is a program in BASIC to count the number of students in the list given below who have scored 70 marks:

Name	Aarti	Akanksha	Manu	Deepak	Anu	Harry	Gunika	Srishti	Manju
Score	72	82	80	70	65	55	85	90	70

```
5 CLS
10 DIM MARKS (___), NAME$(___)
20 FOR I = 1 TO ___
30 READ NAME$(__), MARKS (I)
40 NEXT I
50 DATA AARTI, 72, AKANKSHA, 82, MANU, 80, DEEPAK, 70
55 _____ANU, 65, HARRY, 55, GUNIKA, 85
60 DATA SRISHTI, 90, MANJU, 70
75 COUNT = 0
80 FOR I = 1 TO 9
90 IF MARKS (I) = ___THEN PRINTNAME$(I); "HAS SCORED 70"
95 COUNT = COUNT + 1
100 NEXT I
105 PRINT COUNT; "NUMBER OF STUDENTS HAVE SCORED 70"
110 END
```

Fill in the blanks with appropriate keywords/ numbers/ words to make it work properly. **6**

d) Write a program in BASIC to draw the figure given below:



6

Q4 a) Resolution of Screen 2 in Graphics mode of BASIC is _____. **0.75**

b) Identify which of the following statements, if any are written incorrectly and write their correct form.
i) IF D < A-B THEN 55 ELSE 75
ii) FOR K$ = 1 TO M
iii) DEF FN(T)= T^4 – T^3
iv) ON N$ GOTO 20, 30, "A"
v) IF X*5 < 0 THEN GOTO 70
vi) FOR I = 50 TO 10 STEP 5 **6**

c) Explain the use of **SCREEN**, **VIEW** and **PSET** commands in BASIC language. **6**

d) The variation of rate constant (k) with temperature (T) for a particular reaction was measured over the temperature range 300-500 K and rate constants are given.

T/K	300	350	400	450	500
$k/(dm^3\ mol^{-1}\ s^{-1})$	7.9×10^6	3.0×10^7	7.9×10^7	1.7×10^8	3.2×10^8

Applying the Arrhenius equation

$$k = Ae^{-E_a/RT}$$

On the above data, write a program in BASIC to fit *lnk* and *1/T* on a straight-line using method of least square fit. Calculate and print the values of activation energy (E_a) and pre-exponential factor (A).

Given:

$$Slope = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

$$Intercept = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

6

Q5

a) OOP stands for _____. **0.75**

b) A list of variables is given below. Indicate errors, if any, in each one of them.

(i) MOL-WT
(ii) END
(iii) Rs.
(iv) TUBELIGHT
(v) "CHEM"
(vi) 3$B

6

c) Write a program in BASIC to find the value of the following series up to first n terms (x is in radians) where user will provide n and the angle in degrees. Include the provision of comparing the output value with the result from library function.

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \ldots\ldots - \infty < x < \infty$$

6

d) Write a user-friendly program in BASIC to carry out product of two matrices **X** and **Y**. The dimensions of matrix **X** is 3×2 and while that of matrix **Y** is 2×3. **6**

Q6

a) 1 PB is equivalent to over_____ digital photos per day. **0.75**

b) Describe the following error messages with examples:

(i) Out of DATA
(ii) FOR without NEXT
(iii) Subscript Out of Range

6

c) Write a program in BASIC to calculate the mean and standard deviation for following observations obtained in the determination of the lead content in a soil sample

0.152 ppm, 0.176 ppm, 0.142 ppm, 0.161 ppm, 0.160 ppm **6**

d) Explain the principle behind finding the area under the curve using Simpson's rule. Write a program in BASIC to find the value of the integral using Simpson's rule with n=10

$$\int ydx = \int_0^1 (4x - 2x^2)dx$$

6

Unique Paper Code	:	32177903_OC
Name of the Paper	:	DSE- Applications of Computers in Chemistry
Name of the Course	:	B.Sc. (H) Chemistry
Semester	:	V
Duration	:	3 hours
Maximum Marks	:	75

Instructions for Candidates

1. All questions carry equal marks.
2. Answer ***four*** questions in all.
3. Attempt all parts of a question together.

Q1 a) In any binary number, the rightmost digit is called_____. **0.75**

b) Define the following standard codes.

a) ASCII
b) Unicode
c) ISCII **6**

c) Write the BASIC statement to produce the following effect

(i) One dimensional array to hold 15 items of string data.

(ii) Assign the value of 3.14 to a variable PI.

(iii) Count the length of a string DSE EXAMINATION and store it in a variable

(iv) If variable X has a value greater than 50, then transfer control to the statement number 50, otherwise execute the next statement.

(v) Print "EXAM" in column 5^{th}.

(vi) Define a polynomial y = x*5 **6**

d) Consider a first order reaction: A ⟶ B. Write a program in BASIC to plot the concentration of A and B as a function of time. Given:

$$[A] = [A]_0 \exp(-kt);$$

$$[B] = [A]_0 \left(\frac{k_1}{k_2 - k_1}\right)(e^{-k_1 t} - e^{-k_2 t})$$

Use $[A]_0 = 1$, $k_1 = 1$, $k_2 = 0.00001$. Vary t from 0 to 5 step 0.01. **6**

Q2

a) DOS is a _____operating system. **0.75**

b) Identify and correct the syntax error in the following statements
   (i) LET X = LEFT$(Y$,3)
   (ii) DEF FN(Y)= Y/Y^2
   (iii) ON Z-5 GOTO 10, Y
   (iv) DIMENSION B (-3, -3)
   (v) PRINT LEN$(TEXT$)
   (vi) FOR A$= M TO L STEP 2 **6**

c) Explain the function of following statements in BASIC (Give examples).
   (i) RESOTRE
   (ii) DEF FN
   (iii) GOSUB **6**

d) Explain the Newton Raphson method for finding root of any polynomial. Write a program in BASIC using user defined function for finding the root of the following polynomial equation using Newton Raphson method within the tolerance limit of 10^{-5}. Given equation is

$$x^3-x^2-2x+1=0$$ **6**

Q3

a) Width to height ratio in screen 2 is _____ **0.75**

b) Write the following algebraic expressions in BASIC.
   (i) P = $A\ e^{-kT}$
   (ii) $p = \frac{nRT}{V-nb} - \frac{an^2}{V^2}$
   (iii) $pH = -log_{10}(H^+)$ **6**

c) Given below is a program in BASIC to print the array

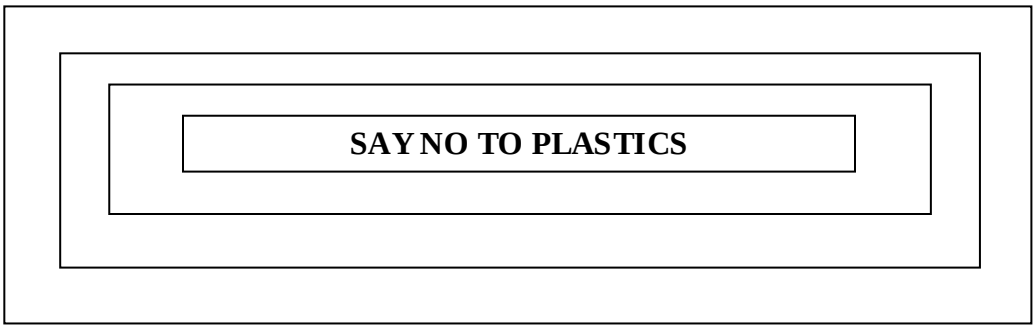
00001
00020
00300
04000
50000

Fill in the blanks with appropriate keywords/numbers/words to make it work properly.

```
10 REM "To write a program to print the given array"
20 INPUT N
30 DIM A(N)
40 PRINT " The Desired Array is"
50 FOR I = 1 TO N STEP 1
60 FOR J = ___ TO N STEP 1
70 IF I = J THEN A(J) = ____ ELSE A(___) = ____
80 NEXT ___
90 FOR K = ____ TO ____ STEP ____
100 PRINT A(___);
110 NEXT ___
120 _____
130 NEXT ___
140 END
```

6

d) Write a program in BASIC to get the following output printed on the screen (four boxes with the slogan Say No to Plastics printed in the middle).



6

Q4 a) An example of common interpreted language is_____. **0.75**

b) Find the error in the following BASIC constants, if any

(i) 1 673%
(ii) 1.6.89!
(iii) Chemistry
(iv) A2
(v) 8939291
(vi) 3.5D98

6

c) What do you understand by hierarchy of BASIC operations? Predict whether the following statement would be true or false, if X = 3 and Y = 5

NOT X < > 3 OR Y < 3 AND X – Y < 0 **6**

d) Write a program in BASIC to evaluate e^x using following series till the contribution $x^n/n!$ is less than 0.0001

$$\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} \ldots\ldots \quad , -\infty < x < \infty$$

6

Q5 a) _____ statement in BASIC is not executed. **0.75**

b) Debug and write the correct form of following programs:

(i)
```
10 DIM P (20,20), DIM Q(20,20)
15 DATA 3,4,5,9
20 FOR I= 2 TO 1
30 FOR J = 2 TO 1
40 READ P I,J
50 Q(I,J) = 10 P(I,J) + J
60 PRINT "Q(I,J) ;
70 NEXT I
80 PRINT
90 NEXT J
```

(ii)
```
20 SCREEN  '640 *480
25 LOCATE (5,25)
30 PRINT  IDEAL GAS ISOTHERMS
40 WINDOW 0,30 – 0.5,400
50 FOR V=0.05 TO 0.5 STEP 0.001
60 P = 0.0821 * T / V
70 PSET V, P
80 NEXT T
90 END
```
6

c) Write a program in BASIC to print the squares of all numbers from 1 to 20 using:
   (i) IF....THEN
   (ii) FOR....NEXT
   (iii) WHILE....WEND

6

d) Write a program to calculate enthalpy for C (s, graphite) from 298K to 500K using Simpson's one-third rule.

$$\int dH = \int_{T_1}^{T_2} C_p dT$$

Given that $C_p = a + bT + \frac{c}{T^2}$ where, a= 16.86, b= 4.77 x 10^{-3}& c= -8.54×10^5.

6

Q6 a) When a loop is present inside another loop, it is called _____ loop. **0.75**

b) Differentiate between the following:
   (i) pre-defined and user-defined functions.
   (ii) GOTO and ON…GOTO statement
   (iii) Define Function and Subroutine

6

c) What are subscripted variables? Write a user-friendly program in BASIC for generating the transpose of a given matrix

$$\begin{matrix} 1 & 0 & 9 \\ 4 & 2 & 7 \\ 5 & 8 & -13 \end{matrix}$$

6

d) The variation of pressure (P) with density (ρ) for a perfect gas is measured at 25°C. The data is shown below.

P/kPa	12.223	25.20	36.97	60.37	85.23	101.3
$\rho/kg\ m^{-3}$	0.225	0.456	0.664	1.062	1.468	1.734

Using the equation $P = \frac{\rho RT}{M}$, write a program in BASIC to fit P and ρ on a straight-line using method of least square fit. Calculate and print Molar mass (M) of the gas.

Given: Gas constant R = 8.314 L kPa mol^{-1} K^{-1}

$$Slope = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

$$Intercept = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

6

Unique Paper Code	:	32177901_OC
Name of the Paper	:	DSE: Novel Inorganic Solids
Name of the Course	:	B.Sc. (Program) Chemistry
Semester	:	V
Duration	:	3 hours
Maximum Marks	:	75

Instructions for Candidate

Attempt four QUESTIONS in all.
All Questions carry equal marks
Question 1 is compulsory

1. **(a)** Fill in the blanks:

(i) …….. is one aspect of the combined electromagnetic force.
(ii) The full form of LCD……..
(iii) Conducting polymers can be obtained from ……reactions.
(iv) CNTs are mainly used as …….. to synthetics.
(v) Cast iron is a …… alloy.

(1.25 x 5 = 6.25)

(b) Answer the following true/false:

(i) The optical properties of liquid crystals depend on the direction of light.
(ii) Due to interactions between molecules, single-molecule magnets stay magnetized even when the magnetic field is turned off.
(iii) Hematite (Fe_2O_3) and magnetite (Fe_3O_4) are the black and red inorganic pigments, respectively.
(iv) Example of magnetic material used in data storage devices is CrO_2.
(v) More than 2% carbon is present in cast irons.

(1.25 x 5 = 6.25)

(c) Answer the following questions in short:

(i) Discuss the role of precipitants in a preparation of metal oxide nanoparticles via co-precipitation method?
(ii) Briefly explain the main characteristics of Polymeric Matrix Composites (PMC) and their engineering applications.
(iii) How does a single molecule behave like a magnet without interacting with each other magnetically?
(iv) Why do black pigments absorb more heat than other colour pigments?
(v) Discuss the liquid crystal electro-optic effect.

(1.25 x 5 = 6.25)

2. **(a)** Describe the reactions that occur during each step of the sol-gel synthesis of inorganic solids utilizing alkoxides as precursors?

(b) Discuss the conduction mechanism of conducting polymer polyacetylene. Also, give its applications.

(c) Define morphosynthesis and describe the relevance of molecular self assembly in fabrication of Nanomaterials.

(6.25 × 3 = 18.75)

3. **(a)** Discuss the main components of fibre reinforced composites. What are the roles of fibre reinforced composites in dentistry?

(b) What are nematic liquid crystals? Describe the various applications of inorganic liquid crystals.

(c) Give the detail of hydrothermal process for the preparation of nanoparticles. Also discuss the use of Teflon in hydrothermal BOMB?

(6.25 × 3 = 18.75)

4. **(a)** Discuss the Ion-exchange resins, their types and applications. In a dual bed system, the cation resin is always first in line why?

(b) What are refractories? Discuss the various types of refractories and their applications with suitable examples.

(c) What are the ceramics? Explain why advanced ceramics have different applications than traditional pottery ceramics?

(6.25 × 3 = 18.75)

5. **(a)** Describe carbon nanotubes and give it's important applications

(b) Discuss the structure and function of Zirconia, ZrO_2 as a solid electrolyte. Also explain "Yttrium Stabilized Zirconia (YSZ)".

(c) What are Silver nanoparticles? Discuss one method of Synthesis of Silver nanoparticles.

(6.25 × 3 = 18.75)

6. Write short notes on ***any three*** of followings:

(i) Super alloys thermoplastics
(ii) Environmental effect of nanocomposite
(iii) Molecular magnet
(iv) One-dimensional metals

(6.25 × 3 = 18.75)

****

Unique Paper Code	: 32347504_OC
Name of the Paper	: Microprocessor (DSE)
Name of Course	: B.Sc. (H) Computer Science
Semester	: V
Duration of Examination	: Three Hours
Maximum Marks	: 75 Marks

Attempt any four questions
All questions carry equal marks

1. Write the steps to program the 8237 DMA Controller. Explain the software commands used to control the operation of 8237 DMA Controller. Find the value of signals A0, A1, A2, A3, $\overline{IOR}$, and $\overline{IOW}$ for the following operations of 8327 DMA Controller command and control port assignments:
   a) Write Request Register
   b) Write Mode Register
   c) Clear Mask Register Bits
   d) Write all Mask Register Bits

   Find the error in each of the following instructions, if any:

   a) LEA OFFSET DX, BX
   b) MUL AL, BL
   c) SUB NUMB, 10H
   d) DEC DI, 2
   e) XLAT AX, BH
   f) MOV SS, CX

2. List the events that occur when an Interrupt becomes active. Differentiate between Real Mode and Protected Mode Interrupt. Describe the operations of the BOUND and INTO instructions.
   Given the contents of sources as TEMP = 01H, BX = 0011H, EAX = 09876543H; find the content of destination register after executing each of the following commands:
   a) MOVZX EBX, TEMP
   b) MOVSX CX, BL
   c) XCHG AX, BX
   d) BSWAP EAX
   e) MOV ECX, 44H

3. Convert the machine language instruction code 67668B048BH into assembly language instruction if it operates in 16-bit instruction mode for 80386 microprocessors and above.

Given DS = 1211H, BX = 0140H, DI = 3000H, ARRAY = 1110H. Determine the data addressing mode and the source address for each of the following instructions in real mode memory addressing:

a) MOV BX, [2200]
b) MOV CX, [BL+4]
c) MOV CX, [EBX+2*EDI]

4. How many clocking periods are there in a Bus Read Cycle and what operations occur during each clocking period in 8088 microprocessor? Explain the operations of 8284A Clock Generator in detail.

   Give the function of the following pins of 8284A Clock Generator:

   a) X_1 and X_2
   b) $\overline{RES}$
   c) F/$\bar{C}$
   d) RDY_1 and RDY_2
   e) PCLK
   f) OSC

5. Contrast the Pentium and Pentium Pro with the 80386 and 80486 microprocessors. Describe the organization and interface of the 64-bit-wide Pentium memory system and its variations. Explain how the superscalar dual integer units improve performance of the Pentium microprocessor.

   Name the Type of Interrupt for the following cases:

   a) Two interrupts occur at the same time.
   b) A logic 1 placed on NMI input pin of the microprocessor.
   c) When an instruction mentions an invalid opcode.
   d) When the overflow condition exists.
   e) The protected mode P bit (P = 0) in a descriptor indicates that the segment is not present or not valid.

6. Explain Mode 1 operation of the 82C55 programmable peripheral interface. Which Port is used for this mode and what bit combination in the Command Byte A register is used to select this mode?

   Differentiate between the two hardware interrupt inputs NMI and INTR. Describe the Initialization Command Words (ICW) for Programmable Interrupt Controller 8259A. Which Operation Command Word (OCW) should be programmed to read the interrupt request register and what should be the required bit values in the OCW for the same?

Unique Paper Code : **32173909 (NC)**
Name of the Paper : **SEC- Pharmaceutical Chemistry**
Name of Course : **B.Sc (Prog)**
Semester: **III/V**
Time Duration : **3 Hours**
Maximum Marks: **38**

Attempt four questions in all. All questions carry equal marks.

1. i) Describe the all stages of drug discovery. Why drug discovery is such a long and costly business, explain?
   ii) Differentiate between the terms Affinity, Efficacy and Potency.

(6,3,5)

2. i) Define the following and give example of each:
   a) Antipyretic agents
   b) Antilaprosy
   c) CNS agents
   d) Cardiovascular agents
   ii) Name various sources of pharmaceutical aids.

(2x4, 1.5)

3. i) Explain different types of fermentation methods. How fermentation process is useful in industrial production of citric acid.
   ii) Define Sulphonamide. Classify them according to their structure.
   iii) Which aspect of pharmacokinetics determines how a drug is administered?

(5,3.5,1)

4. Give method of preparation of any three of the following:
   a) Sulphamethoxazol
   b) Phenobarbital
   c) AZT-Zidovudine
   d) Aspirin

(3.16 x 3)

5. i) Write short note on any two of the following:
   a) Preparation of cephalosporin
   b) Preparation of vitamin B2
   c) Industrial preparation of ethyl alcohol
   ii) What is the goal of Drug therapy?

(3.5 x 2, 2)

6. i) What are the natural sources of Drugs? Give uses and abuses of herbal drugs?
   ii) What was the problem caused by the Drug thalidomide in 1960s?
   iii) What is the difference between Drug and medicine?

(5.5, 2, 2)

Unique Paper Code	:	**42177925**
Name of the Paper	:	**DSE: Chemistry of d-block Elements, Quantum Chemistry and spectroscopy**
Name of the Course	:	**B.Sc. Prog. Life Science**
Semester	:	**V**
Duration	:	**3 hours**
Maximum Marks	:	**75**

Instruction for Candidates

1. Following details to be written on first page:
   University. Roll. No.
   Name:
   Class:
   Course:
   Semester:
   Paper Name:
   Unique paper code:
2. Put page numbers on every page of the answer script
3. Attempt **any two** questions from **each section** (Total four questions)
4. Attempt all parts of a question together.

SECTION A

Q.1.

a) Write down the IUPAC names of the following coordination compounds:

i. $K_3[Fe(CN)_5NO]$

ii. $[(en)_2Co(NH_2)(OH)Co(en)_2](SO_4)_2$

iii. $[Pt(NH_3)_4Cl_2][PtCl_4]$

iv. $[Ni(NH_3)_2(py)(Cl)]$

(2 x 4 = 8)

b) Write down the formula for the following coordination compounds

i) Ammonium tetrachloridoplatinate(II

ii) Potassium carbonyltetracyanido-C-iodidoferrate(III)

iii) Potassium trioxalatoferrate(III) trihydrate

(2 x 3 = 6)

c) Explain *Linkage isomerism* and *coordination isomerism* with the help of examples for each **4¾**

Q.2.

a) VBT fails in predicting the relative stabilities of the complexes $[Co(CN)_6]^{3-}$ and $[Co(NO_2)_6]^{3-}$ while CFT can. Justify.

3

b) Define Jahn Teller distortion. Giving justification, explain which of these configurations d^3, d^4, and d^9 will undergo tetragonal distortion in octahedral ligand field?

6.5

Tetrahedral ligand field splitting is considerably lower than octahedral crystal field splitting. Explain **4**

c) Define inner orbital and Outer orbital complexes giving suitable examples in each case.

5¼

Q.3.

a) Provide a suitable explanation for the following statements:

(i) Transition elements have high enthalpies of atomisation

(ii) Zn^{2+} compounds are white while Cu^{2+} are blue in colour.

4

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

(i) Catalytic properties of transition metals and their complexes

(ii) Advantages of CFT over VBT in coordination compounds.

(iii) Colour and magnetic properties of lanthanides

8

c) The Latimer diagram of Mn in acidic solution is given below:

$$MnO_4^- \xrightarrow{+0.90\ V} HMnO_4^- \xrightarrow{+1.28\ V} H_3MnO_4 \xrightarrow{+2.9\ V} MnO_2 \xrightarrow{+0.95\ V} Mn^{3+} \xrightarrow{+1.5\ V} Mn^{2+} \xrightarrow{-1.18V} Mn$$

(i) Which oxidation states of Mn are unstable w.r.t disproportionation in aqueous medium and why?

(ii) Can Mn(s) be a reducing agent?

(iii) Which of the above species can reduce water to H_2 in acidic medium?

(iv) What is the oxidation state of Mn in $HMnO_4^-$?

6¾

Q.4.

a) What are the photoelectric cell?

2¾

b) What are the auxochrome and chromophore? Explain with examples.

4

c) Find out that function $\phi(x)$ is an eigen function of the given operator ($\hat{A}$) or not. In case of eigen function, give its eigenvalue?

(i) $(\hat{A}) = \frac{d}{dx^2}^2$; $\phi(x) = Cos\ \omega x$

(ii) $(\hat{A}) = \frac{d}{dt}$; $\phi(x) = e^{-i\omega t}$

4

d) The spacing of lines in the microwave spectrum of $^{35}Cl^{19}F$ is 1.033 cm^{-1}; calculate moment of inertia and bond length of the molecule.

4

e) Which of the following molecules may show rotational and vibrational spectra and why?
(i) CH_3CH_3 (ii) CH_4 (iii) CH_3Cl (iv) N_2

4

Q.5.

a) What are the primary and secondary photochemical processes?

2¾

b) What are physical significance of $\psi\ and\ \psi^2$ for a particle in one dimensional box. Sketch the plot of $\psi\ and\ \psi^2$ of "a particle in one dimensional box" for n = 1 to n =5.

4

c) Explain symmetric and asymmetric stretching, and bending modes of molecules with example?

4

d) Derive the expression for the average energy ($\langle E \rangle$) for the particle in one-dimensional box of length *l* using following Wavefunction:

$$\psi_n = \sqrt{\frac{2}{l}} Sin\ \frac{n\pi x}{l} \qquad 0 \le x \le l$$

where n (principal quantum number) = 1, 2…so on

4

e) A solution of an unknown component of a biological sample when placed in an absorption cell of path length 1.00 cm transmits 18.1 percent of light of 320 nm incident upon it. What is the molar absorption coefficient, If the concentration of the component is 0.139 mmol dm^{-3}?

4

Q.6.

a) Define zero-point energy? Why is it not zero in vibrational spectra?

2¾

b) Describe absorption, fluorescence and phosphorescence. Write the increasing trend in the life time of the absorption, fluorescence and phosphorescence and also give its reason.

4

c) How many normal modes of vibration are possible for the following molecules:

(i) C_6H_6 (ii) NO_2 (iii) HC≡C-C≡C-H

4

d) What is the selection rule for the vibrational quantum number? The vibration frequency of $^1H^{35}Cl$ is 2990.6 cm^{-1} . Calculate the bond force constant.

4

e) Find out the value of the following commutators:

(i) $\left[x, \frac{d}{dx}\right]$
(ii) $[x^n, p_x]$

4