

[This question paper contains 3 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 8590  
Unique Paper Code : 32171101  
Name of the Paper : Inorganic Chemistry  
Name of the Course : B.Sc. (H) Chemistry  
Semester : I  
Duration : 3 Hours

J

Maximum Marks : 75

1. Write your roll number on the top immediately on receipt of this question paper
2. Attempt six questions in all.
3. Question number one is compulsory.
4. The questions should be numbered in accordance with the number in the question paper.
5. Calculator and lock tables may be used.

1. Explain any five of the following

- (I) Ionic radii of  $\text{Na}^+$  and  $\text{Cu}^{2+}$  ions are almost similar.
- (II) An electron moving in an orbital does not slow down gradually.
- (III) Electron affinity of Nitrogen is lower than Oxygen.
- (IV) HF is liquid whereas HCl is a gas.
- (V)  $\text{H}_2$  is known while  $\text{He}_2$  is not.
- (VI)  $\text{BeCl}_2$  has zero dipole moment while  $\text{H}_2\text{S}$  has some.

(3x5=15)

2. (I) Draw radial probability distribution curve for  $1s, 4p, 5s, 4d$ . What are radial and angular wave functions?

(II) Drive the Born-Landé's equation for lattice energy of a crystal lattice.

(III) Explain significance of Azimuthal quantum number.

(6, 4, 2)

3. (I) Calculate  $Z^*$  (effective nuclear charge- Slater's rule) for  $2s$  and  $4s$  electrons.

(II) During ionization of atoms having  $ns$  and  $(n-1)d$  electrons, the electron of  $ns$  orbital lost first. Why?

(III) Find out electron gain enthalpy using following data:

Enthalpy of formation :  $382 \text{ KJ mol}^{-1}$

Lattice Energy :  $759 \text{ KJ mol}^{-1}$

Ionization Enthalpy :  $494 \text{ KJ mol}^{-1}$

Dissociation Energy  $\text{Cl}_2$  :  $121 \text{ KJ mol}^{-1}$

Sublimation Energy (Na) :  $108 \text{ KJ mol}^{-1}$

(3, 3, 6)

4. (I) Draw molecular orbital energy level diagram of  $\text{O}_2^-$  and  $\text{NO}^+$ . Which has higher bond energy?

or

Draw molecular orbital energy level diagram of  $\text{NO}^-$  and  $\text{HCl}$ . Which has higher bond energy?

(II) Using VSEPR theory give the shape of  $\text{POCl}_3, \text{SF}_6, \text{BrF}_4^-, \text{NH}_3$ .

(III) What is Fajan's Rule? Explain why lithium halides are covalent in spite of the

5. (I) First ionization energy of Be is greater than Li but position is reversed in case of second ionization energy of Be and Li. Why?

(II) Why P-Nitrophenol has higher boiling point than O-nitrophenol phenol?

(III) Write short note on following (any three)

- a. London or dispersion forces  
 b. Dipole-dipole interaction  
 c. HF is liquid HCl is gas  
 d. Hybridization (3,3,2x3)
6. (I) Explain Conductivity of metals and semiconductors using band theory.  
 (II) What was the velocity of a beam of electron if they are display a de-Broglie wavelength of  $100 \text{ \AA}$   
 (III)  $\psi$  has no physical significance and  $\psi^2$  has. Explain.  
 (IV) Be and N in second period and Mg and P in third period of the periodic table have higher ionization energy than expected. Justify  
 (V) What do you understand by equivalent and non-equivalent hybrid orbital's give one example of each  
 (VI) Bond angle of  $\text{CH}_4$  is higher than  $\text{NH}_3$ . Explain. (2X6)
7. (I) Draw neatly labelled molecular orbital diagram of  $\text{N}_2^-$  and  $\text{O}_2^{2+}$  with bond order and magnetic behaviour .  
 (II) Write Schrödinger equation for Hydrogen atom. Explain terms involved in it and write conditions for physical significance of the equation.  
 (III) What are Slater rules, calculate the  $Z^*$  effective nuclear charge for the valence electrons in G, Z is equal to 31. (4X3)
8. (I) First ionization enthalpy of Oxygen is less than that of Nitrogen. Give reason.  
 (II) Which of following is more covalent and why?

$\text{CuCl}$  or  $\text{KCl}$

- (IV) If a solid " $\text{A}^+\text{B}^-$ " has a structure similar to  $\text{NaCl}$ . Consider the radius of anion as  $250 \text{ pm}$ . Find the ideal radius of the cation in the structure. Is it possible to fit a cation  $\text{C}^+$  of radius  $180 \text{ pm}$  in the tetrahedral site of the structure " $\text{A}^+\text{B}^-$ "?  
 (3,2,2,5)

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Roll No.

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S. No. of Question Paper : 8610

Unique Paper Code : 32171102

J

Name of the Paper : Physical Chemistry - I

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

Semester : I

Duration : 3 Hours

Maximum Marks : 75

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

Attempt six questions in all.

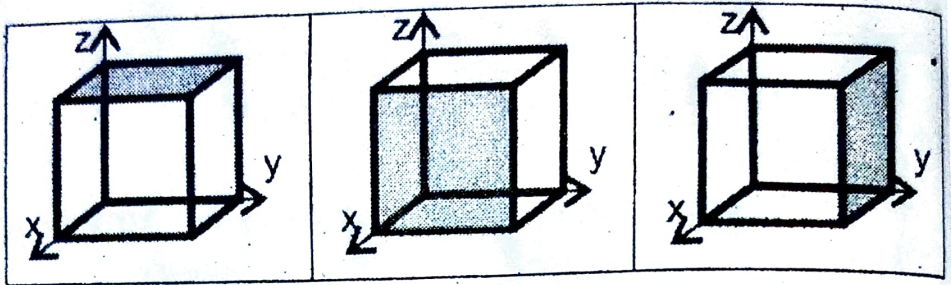
Question No. 1 is compulsory.

Use of scientific calculator and log tables is permitted.

1. Explain briefly, any five statements of the following :
  - (a) An ideal gas is not expected to show any cooling on free expansion.
  - (b) Addition of detergents decreases the surface tension of water.

P.T.O.

- (c)  $K^+$  ions and  $Cl^-$  ions are indistinguishable by X-ray diffraction.
- (d) Identify the type of lattice planes shown in the following figures :



i

ii

iii

- (e) The viscosity of gas increases with temperature while that of liquid decreases with temperature.
- (f) Can pH of an aqueous solution be less than 0 or more than 14 at  $25^\circ C$  ?
- (g) Phenolphthalein is not a suitable indicator for a strong acid-weak base titration.

5×3

2.

- (a) Starting from the postulates of kinetic theory of gases, derive the Kinetic Gas Equation  $pV = \frac{1}{3}mN\bar{u}^2$ , where symbols have their usual meaning.
- (b) What is law of corresponding states ? Derive the reduced equation of state for van der Waals equation of state.

- (c) The critical constants for water are 647 K, 22.09 MPa and  $0.0566 \text{ dm}^3 \text{ mol}^{-1}$ . Calculate the values of van der Waals constants  $a$ ,  $b$  and  $R$  and also explain the abnormal value of  $R$ . 4,4,4
- (a) Write the mathematical expression for the Maxwell distribution of molecular speeds for a gas and explain briefly the terms involved. Derive the mathematical expression for the most probable speed of a gas molecule.
- (b) The mean free path of molecules in a gas increases and the number of collisions per unit time decreases with lowering of pressure if temperature is kept constant. Explain.
- (c) The average speed at  $T_1$  K and most probable speed at  $T_2$  K of  $\text{CO}_2$  is  $9 \times 10^2 \text{ m s}^{-1}$ . Calculate the value of  $T_1$  and  $T_2$ . 5,3,4
- (a) Describe the powder diffraction method to determine crystal structure. Explain the significance of missing lines in the analysis of crystal structure using powder diffraction method.

- (b) Evaluate the Miller indices for the planes following intercepts :
- (i)  $0a, 2b, 2c$
- (ii)  $a, 1/3b, 1/4c$
- (iii)  $-2a, 3b, 4c$
- (c) Show that a 5-fold rotation axis of symmetry can't exist in a crystal.
5. (a) How does viscosity of a liquid vary with temperature? Give the mathematical expression of the same for each term.
- (b) Define surface tension of liquid and give its SI unit. Describe a method for its experimental determination.
- (c) If the flow time for the two liquids A and B through the same capillary is in the ratio of 4 : 5 and the radii are in the ratio of 2 : 1. What is the ratio of their viscosities ?
6. (a) Show that the concentration of  $H_3O^+$  in an aqueous solution of a monoprotic acid HA can be computed from the following expression :

$$K_a = \frac{[H_3O^+]^3 - [H_3O^+]K_w}{[H_3O^+][HA]_0 - [H_3O^+]^2 + K_w}$$

Under what conditions can the following expressions be used :

$$K_a = \frac{[\text{H}_3\text{O}^+]^2}{[\text{HA}]_0 - [\text{H}_3\text{O}^+]}$$

$$K_a = \frac{[\text{H}_3\text{O}^+]^2}{[\text{HA}]_0}$$

- (b) Define different types of buffer solutions. Derive Henderson-Hasselbalch equation for pH of acidic and basic buffer.
- (c) What is pH of a solution obtained by mixing 50 mL, 0.1M HCl with 50 mL, 0.1 M  $\text{NH}_4\text{OH}$ . (Given :  $\text{pK}_b$  of  $\text{NH}_4\text{OH}$  = 4.74). 4,4,4

7. (a) Define solubility and solubility product. Express solubility product of the given salts in terms of the solubility of ions :



(b) Show that the pH of an aqueous solution of salt formed from a strong acid and weak base is given by :

$$\text{pH} = 7 - \frac{1}{2}(\text{pK}_b + \log c)$$



(c) Will a precipitate form if equal volumes of 0.01 M  $\text{AgCl}$  and 0.0004 M  $\text{NaCl}$  are mixed ? Given  $K_{sp}$  of  $\text{AgCl}$  is  $1.7 \times 10^{-10} \text{ M}^2$ .

8. (a) Write the van der Waals equation in the virial form and evaluate the second virial coefficient.

(b) Calculate the volume occupied by 2.0 mol of  $\text{N}_2$  at 300 K and 10.1325 MPa pressure if  $p_r V_r / T_r$  is equal to 2.0.

(c) Calculate at  $25^\circ\text{C}$  the exact pH of a solution of (a) 0.01 M  $\text{NaOH}$ , and (b)  $10^{-7}$  M  $\text{NaOH}$ . 4,4

9. Write short notes on any four :

(i) Law of equipartition of energy

(ii) Rotating crystal method

(iii) Theory of Acid-base indicators

(iv) Continuity of States

(v) Cleansing action of detergents. 4x

[This question paper contains 4 printed pages]

**Your Roll No.** : .....

**Sl. No. of Q. Paper** : **7393**      **J**

Unique Paper Code : 32171301

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

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

Semester : III

**Time : 3 Hours**                      **Maximum Marks : 75**

**Instructions for Candidates :**

- (i) Write your Roll No. on the top immediately on receipt of this question paper.
- (ii) Attempt any **five** questions.
- (iii) All questions carry equal marks.

1. (a) Explain why most lines in the Ellingham diagram slope upward from left to right. What happens when a line crosses  $\Delta G=0$  ?      5

(b) Why is white phosphorus very reactive in comparison to red phosphorus ? Give the mechanism of stepwise hydrolysis of  $P_4O_{10}$ .  
5

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- (c) How will you obtain the following :
- B-bromoborazine from borazine
  - $(\text{NPF}_2)_3$  from  $(\text{NPCl}_2)_3$
2. (a) Chemistry of Lithium is different from other alkali metals. Give examples in support of the statement.
- (b) What are clathrate compounds of noble gases? Why do helium and neon not form clathrates?
- (c) Give one method of preparation of peroxodisulphuric acid. What is the oxidation state of Sulphur in it? Give one reaction in support of its strong oxidizing nature.
3. (a) Name the class of silicates present in the following minerals. Write the basic silicate unit present in them and give their structures.
- Zircon
  - Emerald or Beryl.
- (b) Among the alkaline earth metals (except Beryllium), which will (a) have the most insoluble sulfate; (b) be the softest metal? Give reason.

(c) Discuss the structure and bonding in Diborane. What are the products formed when diborane reacts with excess ammonia at

5

- (i) low temperature
- (ii) high temperature

4. Give reason (**any five**) :

3×5=15

- (i)  $P_4$  molecule is more stable than the  $P_2$  molecule.
- (ii) Ionization energy decreases from B to Al but increases from Al to Ga.
- (iii)  $H_2O$  a liquid but  $H_2S$  a gas at room temperature.
- (iv) Only the alkali metals form solid, stable hydrogen carbonate salts.
- (v) The bond angle in  $NH_3$  is  $107^\circ$  while in  $PH_3$  is  $93^\circ$ .
- (vi) Interhalogens are more reactive than the halogens.

5. (a) Explain briefly the complex formation tendency of the alkali metals with special reference to crown ethers and cryptands.

5

(b) (i) What are pseudohalogen compounds ?

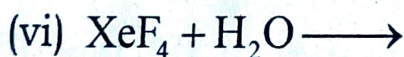
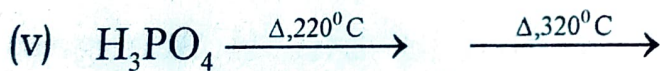
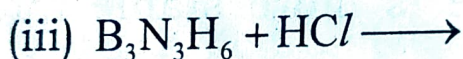
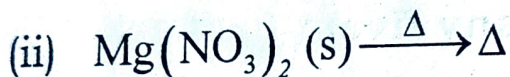
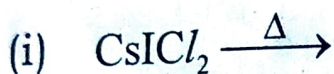
2.5

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(ii) Draw the structure of the following compounds:

$\text{ICl}_3$ ,  $\text{H}_2\text{SO}_5$ , Basic Beryllium acetate

(c) Complete the following (any **five**):



6. Write short notes on (any **three**):

5×3=15

(a) Allotropes of Carbon

(b) Hydrometallurgy

(c) Inert pair effect

(d) Craig and Paddock model for imperfect delocalization of  $\pi$ -electrons in  $(\text{NPCl}_2)_3$ .

[This question paper contains 4 printed pages]

Your Roll No. : .....

Sl. No. of Q. Paper : 7394 J

Unique Paper Code : 32171302

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

Name of the Paper : C VI - Organic Chemistry - II

Semester : III

Time : 3 Hours Maximum Marks : 75

**Instructions for Candidates :**

- (a) Write your Roll No. on the top immediately on receipt of this question paper.
- (b) Attempt any **five** questions.
- (c) **All** questions carry equal marks.

1. (a) An organic compound A ( $C_9H_{10}O$ ) reacts with iodine and aq. Sodium hydroxide to give iodoform and sodium salt of an acid B ( $C_8H_8O_2$ ). B on reaction with chlorine and red phosphorous forms compound C ( $C_8H_7O_2Cl$ ). Hydrolysis of C followed by acidification gives compound D. Identify A, B, C, & D with the reactions involved. Name the reaction by which B is converted to C. Write the mechanism for conversion of A to B.

10

P.T.O.

(b) Write one test along with reaction involved for distinction between the following pairs of compounds : 2.5×2=5

- (i) 1-Pentanol and 2-pentanol
- (ii) Acetaldehyde and benzaldehyde

2. How will you prepare the compounds a, b, & c from ethyl acetoacetate and d & e from diethyl malonate ? 3×5=15

- (a) 3-Methylpentan-2-one
- (b) Succinic acid
- (c) 2-Methylhexanoic acid
- (d) Cinnamic acid
- (e) 5-Ethylbarbituric acid

Explain the following : 3×5=15

- (a) The rate of hydrolysis of the carboxylic acid derivatives is  

$$\text{CH}_3\text{COCl} > (\text{CH}_3\text{CO})_2\text{O} > \text{CH}_3\text{CONH}_2.$$
- (b)  $\text{S}_{\text{N}}1$  reactions are accompanied by racemization as well as inversion of configuration.
- (c) *o*-Nitrophenol is a weaker acid than *p*-nitrophenol.
- (d) Reactivity of aryl halides towards nucleophilic substitution increases with the substitution of nitro group at *ortho*- and *para*-positions.

(e) t-Butyl methyl ether is prepared by reaction of methyl chloride and sodium t-butoxide rather than from t-butyl chloride and sodium methoxide.

4. Write the products for the following along with equations : 3×5=15

(a) When oxalic acid, succinic acid and adipic acid are heated separately.

(b) Ethyl acetate is treated with sodium ethoxide followed by reaction with one mole of ethyl iodide in the presence of sodium metal.

(c) Phenol is heated with carbon dioxide under pressure in the presence of sodium hydroxide followed by reaction with acetic anhydride in the presence of acid catalyst.

(d) Acetone when reacted with hydroxyl amine followed by treatment with Conc.  $H_2SO_4$ .

(e) Maleic acid and fumaric acid are treated separately with dil.  $KMnO_4$ .

5. How will you carry out the following conversions ? 3×5=15

(a) Ethanoic acid to Propanoic acid

(b) Benzene to ethoxybenzene

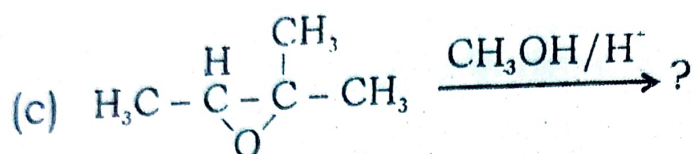
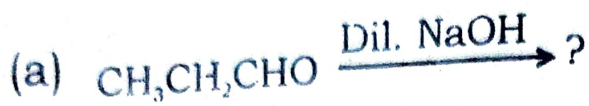
(c) Acetone to 2-methyl-2-butanol

(d) Benzaldehyde to benzamide

(e) Aniline to fluorobenzene



6. Complete the following reactions. Write the mechanism of the reaction involved. Write the  
5×3=15



7. Write short notes on any **three** of the following with emphasis to (i) the functional group that undergoes these reactions, (ii) products formed (iii) reaction conditions and (iv) mechanism.

5×3=15

- (a) Baeyer-Villiger oxidation
- (b) Cannizzaro reaction
- (c) Fries rearrangement
- (d) Benzil-benzilic acid rearrangement
- (e) Michael addition

[This question paper contains 7 printed pages]

Your Roll No. : .....

Sl. No. of Q. Paper : 7395 J

Unique Paper Code : 32171303

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

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

Semester : III

**Time : 3 Hours**                      **Maximum Marks : 75**

**Instructions for Candidates :**

- (a) Write your Roll No. on the top immediately on receipt of this question paper.
- (ii) Question No. 1 is compulsory.
- (iii) Attempt **six** questions in all, selecting at least **two** questions from each Section.
- (iv) Use of scientific calculator is allowed.

Values of constants :

$$R=8.314 \text{ J K}^{-1} \text{ mol}^{-1},$$

$$F=96500 \text{ C mol}^{-1}, (2.303 RT/F) \text{ at } 298 \text{ K} = 0.0591$$

P.T.O.

7395

1. Explain (any **five**) :

3×5=

- (a) How can liquid junction potential be eliminated ?
- (b) Quinhydrone electrode is not suitable for measurement more than 8.5.
- (c) Difference between electrolytic and galvanic cell.
- (d) Use of adsorbent in powdered form.
- (e) Slope of fusion curve of water system is inclined towards pressure axis.
- (f) Plait point lies either to the left or right of the maximum of the binodal curve in a three component system.
- (g) Triethylamine-water system shows low CST.

### Section - A

2. (a) Derive phase rule for a non-reactive system

(b) Show that  $\text{NH}_4\text{Cl}(\text{s}) - \text{NH}_3(\text{g}) - \text{HCl}(\text{g})$  system in which  $P_{\text{NH}_3} = P_{\text{HCl}}$  is a one component system whereas when  $P_{\text{NH}_3} \neq P_{\text{HCl}}$  is a two component system. 4

(c) The vapour pressure of toluene is 59.1 torr at 313.75K and 298.7 torr at 353.15K. Calculate the molar heat of vaporization. 4

3. (a) Differentiate between congruent and incongruent melting point system with an example. 4

(b) Metal A and B melts at  $110^\circ\text{C}$  and  $75^\circ\text{C}$  respectively. They form one compound  $\text{A}_2\text{B}$  which decomposes at  $20^\circ\text{C}$  to give a solid and a melt containing 50mole % of B. There is a eutectic point at  $5^\circ\text{C}$  and eutectic composition is 70 mole % of B. Sketch the phase diagram and label it. 4

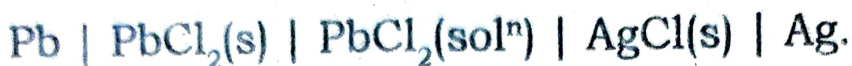
(c) Show that multistage extraction is more economical than single stage extraction. 4

4. (a) Derive Duhem Margules equation applicable to a binary liquid mixture and show that if one component behaves ideally then other component also behaves ideally.
- (b) Calculate the degree of freedom at a point which lies anywhere :
- Outside the binodal curve
  - Within the binodal curve
- (c) Write a short note on fractional distillation.
5. (a) State and derive the lever rule.
- (b) Draw a well labelled phase diagram for chloroform-acetic acid-water system.
- (c) The vapour pressure of aniline and water at  $98.5^{\circ}\text{C}$  are 717 mm and 43 mm respectively. Molar masses of liquids are 93 and 18. Calculate the relative masses of two liquids in the distillate after the steam distillation.

### Section - B

6. (a) How will you determine the accurate value of half-cell potential graphically?

(b) For the following cell : 4



The potential at 298K is 0.490V and the variation of emf with temperature is given by :

$$E = a - (1.86 \times 10^{-4} \text{VK}^{-1})(T - 25\text{K})$$

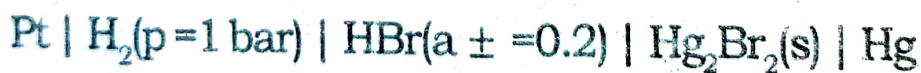
Calculate  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  for the reaction at 298 K.

(c) Describe the construction of hydrogen electrode along with necessary diagram and chemical equations. Give its limitation also.

4

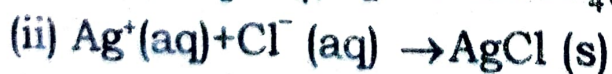
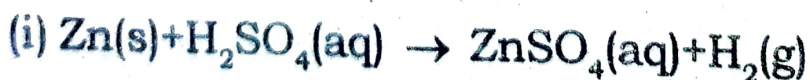
7. (a) What are concentration cells ? Derive the expression for a concentration cell with transference. 4

(b) Calculate the cell potential at 25°C for the cell : 4



Given  $E^0_{\text{Br}^- \mid \text{Hg}_2\text{Br}_2 \mid \text{Hg}} = 0.1385\text{V}$

(c) Construct the galvanic cell for the following reactions and write the expression for the cell potential 4



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8. (a) Explain :

(i) Why chemisorption is monolayer and physisorption is multilayer.

(ii) Most adsorption processes are exothermic in nature.

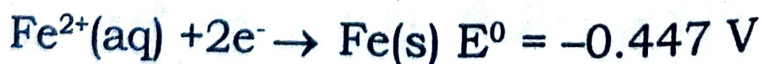
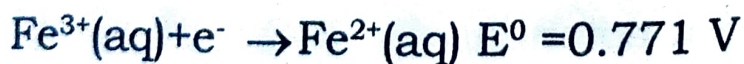
(b) Derive the following Langmuir Adsorption isotherm :

$$\frac{p}{x/m} = \frac{1}{k_1 k_2} + \frac{p}{k_2}$$

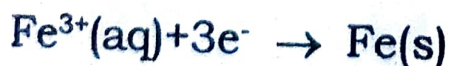
Explain the various symbols.

(c) From the following reduction reactions and

$E^0$  values :



Calculate  $E^0$  for the half-cell reaction



7395

9. Write short note (any **three**) :

4×3=12

- (i) Potentiometric titrations
- (ii) Reversible and irreversible galvanic cells
- (iii) Different types of half cells
- (iv) Glass electrode



[This question paper contains 4 printed pages]

**Your Roll No.** : .....

**Sl. No. of Q. Paper** : **7396**      **J**

Unique Paper Code : 32171501

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

Name of the Paper : Organic Chemistry - IV

Semester : V

**Time : 3 Hours**

**Maximum Marks : 75**

**Instructions for Candidates :**

- (a) Write your Roll No. on the top immediately on receipt of this question paper.
- (b) Question No. **1** is compulsory.
- (b) Attempt **six** questions in all.

**1.** Answer any **five** of the following :       $3 \times 5 = 15$

(a) The sequence ACGTGC (reading in the  $5' \rightarrow 3'$  direction) appears on a portion of one strand of DNA. What is the corresponding sequence on the complementary strand of the DNA double helix? Show the polarity of this complementary strand.

(b) (i) Show which nitrogen atom of histidine heterocycle is basic and which is not.

(ii) Show the structure that results when histidine accepts a proton on the basic nitrogen and then is deprotonated on the other heterocyclic nitrogen.

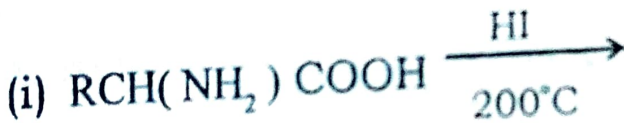
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- (c) Explain the term "anabolism" and give an example.
- (d) For lysine, the  $pK_a$  values of  $\alpha$ -carboxyl, the  $\alpha$ -amino, and the side chain amino groups are 2.2, 9.1 and 10.5 respectively. Write down the structure of lysine at its  $pI$  and calculate its  $pI$  value.
- (e) Explain the following terms and give an example :
- (i) Bactericide      (ii) Bacteriostatic
- (f) What is "iodine number" ? What is its significance ?
2. (a) Convert :
- (i) Cytosine  $\rightarrow$  5-Nitrocytosine
- (ii) Urea  $\rightarrow$  Uracil
- (b) Give synthesis of Cytosine from malondialdehyde acetal.
- (c) Write down the systematic name and structures of :
- (i) Cytidine      (ii) Guanosine
3. (a) Write the structure and name of coenzyme formed from vitamin Riboflavin .
- (b) Classify the following enzymes according to the type of reaction that they catalyze. Give the first digit of E.C.number.
- (i) Phosphotriose isomerase
- (ii) Phosphofructo kinase
- (c) Differentiate between competitive and noncompetitive inhibition.

4. (a) Give synthesis of Chloramphenicol from p-Nitroacetophenone. Write the name of compound used for resolution.
- (b) (i) Is chloramphenicol bactericide or bacteriostatic? Explain it through its mode of action.
- (ii) What are antipyretics? Give an example.
- (c) Vitamine C is required for synthesis of structural protein of skin, connective tissue. Name the protein. Give the name of disease caused by severe deficiency of Vitamine C.

4×3=12

5. (a) Complete the following reactions :



- (b) Treatment of a protein with trypsin gave a peptide 'A' which on complete hydrolysis produced :

Ser, Ala, Gly, Phe, Val, Lys, Asp

Partial hydrolysis of 'A' with Chymotrypsin gave a dipeptide and a pentapeptide. On treatment with sanger's reagent followed by hydrolysis, the dipeptide gave DNP-Asp. The pentapeptide was cycled through Edman's degradation three times. The composition of the peptide remaining after each cycle was as follows :

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Cycle 1 : Ala, Lys, Ser, Gly

Cycle 2 : Ala, Lys, Gly

Cycle 3 : Ala, Lys

What is the sequence of amino acids in the heptapeptide ? Explain all the reactions.

6. (a) Write down two irreversible steps of citric acid cycle. Write all the structures and name of enzymes.
- (b) How is pyruvate converted into lactate under anaerobic conditions ? Write down all the reactions involved. Give the name of enzymes also.
- (c) Give Solid phase synthesis of the tripeptide Gly, Ala, Val 4×3=12
7. (a) Explain the term "Rancidity" of oils. How can it be prevented.
- (b) What is acid value of an oil ? What is its significance ?
- (c) How many grams of KOH would be required to neutralise a suspension in water of 250g of fat whose acid value is 40. 4×3=12
8. Write down short notes on any **three** of the following : 4×3=12
- (i) Allosteric enzymes
  - (ii) Factors affecting enzyme action
  - (iii) Secondary structure of proteins
  - (iv) Electrophoresis

[This question paper contains 8 printed pages]

Your Roll No. : .....

Sl. No. of Q. Paper : **7397**      **J**

Unique Paper Code : 32171502

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

Name of the Paper : Physical Chemistry - V :  
Quantum Chemistry and  
Spectroscopy

Semester : V

**Time : 3 Hours**      **Maximum Marks : 75**

**Instructions for Candidates :**

- (i) Write your Roll No. on the top immediately on receipt of this question paper.
- (ii) Attempt any **six** questions in all.
- (iii) Question No. **1** is compulsory. Each part of Question No. **1** carries **3** marks.
- (iv) Each part of the rest of the questions carries **4** marks.
- (v) Attempt all parts of a question together.
- (vi) Use of scientific calculators is allowed but they cannot be shared.
- (vii) Logarithmic tables can be provided if required.

P.T.O.

### Physical Constants

Planck's constant	$6.626 \times 10^{-34} \text{ Js}$
Velocity of light	$3 \times 10^8 \text{ ms}^{-1}$
Avogadro's number	$6.023 \times 10^{23}$
Mass of electron	$9.1 \times 10^{-31} \text{ kg}$
Nuclear Magneton	$5.05 \times 10^{-27} \text{ JT}^{-1}$
Bohr Magneton	$9.27 \times 10^{-24} \text{ JT}^{-1}$
Boltzmann Constant	$1.38 \times 10^{-23} \text{ JK}^{-1}$

1. Attempt any **five** of the following :
- How will the rotational spectra change when  $^{12}\text{C}$  in  $^{12}\text{C}^{16}\text{O}$  is replaced by  $^{13}\text{C}$  ?
  - Write the Hamiltonian for  $\text{H}_2$  molecule and explain each term.
  - The term 'state' and 'energy level' are not synonymous in wave-mechanics. Explain. How many states and energy levels lie in the energy range of  $E < 10h^2/8ml^2$  ?
  - The function given below are defined in the interval  $x=-a$  and  $x=+a$  as follows :  

$$f(x) = N (a^2 - x^2)$$
 Assuming the value of the function to be zero for  $x < -a$  and  $x > +a$ , calculate the Normalization constant  $N$ .
  - 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  $k = 2Da^2$ .

- (f) What are the essential conditions for a molecule to show IR Spectra. Which of the following will be IR active :  $O_2$ ,  $CO_2$ ,  $CO$  and  $SO_2$ .
- (g) Homonuclear diatomic molecule,  $Br_2$ , is microwave inactive but is rotational Raman active. Why ?

2. (a) Show that the probability of finding the particle in a one-dimensional box in the region  $L/4$  and  $3L/4$  is  $1/2$  if  $n$  is even, and

$$\frac{1}{2} + \frac{(-1)^k}{n\pi} \text{ if } n \text{ is odd.}$$

- (b) A particle of mass  $m$  moves in a three-dimensional box of sides  $a$ ,  $b$ ,  $c$ . If the potential is zero inside and infinity outside the box, give the expressions for the energy eigenvalues and wavefunctions for a particle in a 3-D box. What is the zero point energy of the system ? What is the degeneracy of the first and second excited states ?
- (c) Evaluate the expectation values of  $\langle x \rangle$  and  $\langle p \rangle$  for the ground state of the harmonic oscillator.

Given : Normalized wavefunction :

$$\Psi \left( \sqrt{\frac{a}{\pi}} \right)^{1/2} e^{-ax^2/2};$$

Standard integral :  $\int_{-\infty}^{\infty} x^2 e^{-ax^2} \cdot dx = \left( \frac{1}{2a} \right) \left( \frac{\pi}{a} \right)^{1/2}$

3. (a) For a one-electron homonuclear diatomic molecule the values of some relevant integrals are given below :

$$\int \Phi_A \hat{H} \Phi_A d\tau = -3 \text{ a.u.} \quad \int \Phi_B \hat{H} \Phi_B d\tau = -3 \text{ a.u.}$$

$$\int \Phi_A \hat{H} \Phi_B d\tau = -3/2 \text{ a.u.} \quad \int \Phi_A \Phi_B d\tau = 1/2$$

where  $\Phi_A$  and  $\Phi_B$  are the normalized set basis functions for an LCAO wavefunction. Find the energy of the bonding molecular orbital and find the normalized wavefunction.

- (b) Calculate the average distance of the electron from the nucleus of H atom in the 2s state.

$$\Psi_{200} = \left( \frac{1}{\sqrt{32\pi}} \right) \left( \frac{1}{a_0} \right)^{3/2} \left( 2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$

$$\left( \text{Given : } \int_0^{\infty} r^n e^{-ar} \cdot dr = \frac{n!}{(a)^{n+1}} \right)$$

- (c) What do you understand by the term transition probability? Depict the energy levels and probability densities for the first four levels of a harmonic oscillator with the help of a diagram.



4. (a) Show that if two operators  $\hat{A}$  and  $\hat{C}$  are Hermitian, then their product ( $\hat{A} \hat{C}$ ) is also Hermitian if and only if  $\hat{A}$  and  $\hat{C}$  commute.
- (b) Write down the normalized Valence Bond wavefunction and Molecular Orbital wavefunction for  $H_2$  molecule. Compare the expressions obtained and explain configuration interaction.
- (c) Arrive at the following expression for  $H_2^+$  :

$$E_+ = \frac{\alpha + \beta}{1 + S}$$

(where  $\alpha$  is the coulomb integral,  $\beta$  is the resonance integral and  $S$  is the overlap integral) using LCAO-MO treatment.

5. (a) The pi electrons of a conjugated molecule can be regarded as moving in a particle in a box, where the box length is somewhat more than the length of the conjugated chain. For butadiene, take this length as 7.0 Å and estimate the wavelength of the light absorbed when a pi-electron is excited from the highest occupied to the lowest vacant level. The experimental value is 217 pm.

- (b) Find the commutator of position and momentum operator and give its physical significance, giving the name of the principle it verifies.
- (c) Gilliam et al. (1950) measured the first line in the rotational spectrum of CO as  $3.8423 \text{ cm}^{-1}$ . Calculate the rotational constant, moment of inertia and find out which rotational state of CO would be most populated at 300 K?
6. (a) What are the selection rules for observing IR spectra of an anharmonic oscillator? Derive the expressions for energy required for fundamental transition and first overtone.
- (b) Dissociation energy of  $^{12}\text{C}^{16}\text{O}$  is  $1.107 \times 10^6 \text{ J mol}^{-1}$ . The anharmonicity constant of the molecule is  $5.860 \times 10^{-3}$ . Find :
- equilibrium frequency of vibration
  - force constant of the molecule
- (c) The line spacing (on each side of the band origin  $\omega_0$ ) in PR spectrum of  $\text{CO}_2$  is  $4B$  instead of the usual  $2B$  as observed in case of HCN. Briefly explain.

7. (a) A molecule  $A_2B_2$  shows IR and Raman spectra as tabulated below :

$cm^{-1}$	IR	Raman
3374	-	strong, polarized
1974	-	strong, polarized
3287	Active (PR)	-
612	-	weak, polarized
729	Active (PQR)	-

Predict the shape of the molecule and assign the various observed lines to the appropriate normal modes of vibrations.

- (b) Show that the separation between the maximum in P and R branches of a vibration rotation spectrum of a heteronuclear diatomic molecule is approximately given as :

$$\Delta\nu = \sqrt{\frac{8kTB}{hc}}$$

where the symbols have their usual meanings.

- (c) Distinguish between Fluorescence and Phosphorescence.

8. (a)  $r_{eq}''$  and  $r_{eq}'$  are internuclear distance of a diatomic molecule in the ground and excited states respectively. Three cases arise :

$$r_{eq}'' = r_{eq}', \quad r_{eq}'' > r_{eq}' \quad \text{and} \quad r_{eq}'' \gg r_{eq}'$$

Discuss the intensity distribution in absorption spectra of any **two** cases using Franck Condon principle along with potential energy diagrams.

- (b) Of the two molecules,  $N_2$  and  $O_2$ , which will show an ESR spectrum and why? Show the hyperfine structure of Methyl radical ( $\cdot CH_3$ ) in ESR spectrum, giving the intensities of the peaks.
- (c) (i) In a spectrometer operating at 1 T, the NMR frequency of  $^{19}F$  is 40.06 MHz. Calculate its magnetogyric ratio/gyromagnetic ratio.
- (ii) Show the low and high resolution NMR spectrum of acidified ethanol.

9. Write short notes on (any **three**) :

- Born Oppenheimer Approximation
- Variation Principle
- Dissociation and Predissociation
- Larmor Precession

No. of Q. P. : 7868  
Unique Paper Code : 32177903  
Name of the Paper : Applications of Computers in Chemistry  
Name of the Course : B. Sc. (H) Chemistry  
Semester : V  
Duration : 03 hours  
Maximum Marks : 75 Marks

J

**Instructions for Candidates**

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

**Question No. 1 is compulsory.**

Attempt **Six** questions in total.

Attempt all parts of a question together.

Answer all parts of the question:

[3 × 5 = 15]

(a) Write the syntax of the following string functions in QBASIC (Attempt any three):

- (i) MID\$
- (ii) INSTR
- (iii) VAL
- (iv) LEN

(b) Write the full form of the following (Attempt any three):

- (i) PIXEL
- (ii) ASCII
- (iii) SSD
- (iv) VDU

(c) Write BASIC expression for the following equations (Attempt any three):

- (i)  $K = \frac{[a]^2}{[b][c]}$
- (ii)  $N = N_0 e^{kt}$
- (iii)  $X = \left[ \frac{(2v+1)hv}{k} \right]^{1/2}$
- (iv)  $C_p = A + BT + CT^2$

(d) Identify the errors in the following (Attempt any three):

- (i) 50,890
- (ii) C\$1 = "HEY"
- (iii) 5.6E-50
- (iv) NEWS.PAPER

(e) Convert  $(11000100)_2$  to hexadecimal and octal number.

2. Attempt all parts.

(a) Identify the errors in the following statements:

- (i) PRINT N: M
- (ii) MOLECULAR \* LEVEL=71
- (iii) A& =1E-07
- (iv) 25,000= \$\$

(b) Differentiate between the following:

- (i) First Generation and Second Generation of Computers
- (ii) Assembly and Machine Language

(c) Write a program in BASIC to determine whether a given number is Prime or not.

3. Attempt all parts.

(a) (i) Write the syntax of the following commands with one example:

- a. PSET
- b. LINE

(ii) Write a program to draw an ARC starting from 0 and ending at  $\pi/2$ .

(b) Write the following programs in BASIC (Attempt any two):

- (i) Draw four concentric circles with origin at (100, 100) in SCREEN 2.
- (ii) Draw a triangle with a point at the centre in SCREEN 1.
- (iii) Draw a rectangle with a diagonal line at the centre in SCREEN 1.

(c) Differentiate between WINDOW and WINDOW SCREEN statement with the help of an example.

4. Attempt all parts.

(a) The viscosity of ether varies with temperature as follows:

T/°C	0	10	30	50	70
$\eta$ /millipoise	3.32	2.85	2.10	1.71	1.18

Write a program in BASIC to determine the value of activation energy (E) of viscous flow using equation:

$$\ln(\eta/\eta_0) = \ln(A/\eta_0) + E/RT$$

Given that:

$$\text{Slope} = (N\sum x_i y_i - \sum x_i \sum y_i) / (N\sum x_i^2 - (\sum x_i)^2)$$

$$\text{Intercept} = (\sum x_i^2 \sum y_i - \sum x_i y_i \sum x_i) / (N\sum x_i^2 - (\sum x_i)^2)$$

(b) What is VIRUS? Also, explain the meaning of the following error messages:

- (i) READ without DATA
- (ii) OUT OF DATA

(c) (i) Write a program in BASIC to print the following output using A\$= "APPLICATIONS OF COMPUTERS IN CHEMISTRY".

APPLICATIONS OF COMPUTERS

IN CHEMISTRY

(ii) What is the significance of REM statement?

Attempt all parts.

(a) Identify the errors in the following program:

```
10 INPUT N$
20 FOR I = 1 TO SQRT(N)
30 R = I MOD N
40 IF R = 0 THEN PRINT N: "N IS A PRIME NO."
50 NEXT K
60 IF R >= 0 THEN 90
70 PRINT N: "N IS A PRIME NO."
80 STOP
```

(b) Write a program in BASIC to determine the roots of the given equation using iterative method:

$$x^5 + 10x - 3 = 0$$

(c) (i) Give the difference between TAB and LOCATE command.

(ii) Give the advantages of High level languages. Name one high level language.

[4 × 3 = 12]

6. Attempt all parts.

(a) Write the output of the following programs:

```
(i) 10 PRINT "hello",
    20 GOSUB 100
    30 PRINT "please",
    40 GOSUB 200
    50 PRINT "thank",
    60 GOSUB 300
    70 PRINT "!!!!!! good bye !!!!!!"
    80 END
    100 PRINT "friend"
    110 RETURN
    200 PRINT "come in"
    210 RETURN
    300 PRINT "you"
    310 RETURN
```

```
(ii) 10 READ A, B, C, D, E, F
    30 DATA 1, 3, 5, 7, 9, 11
    40 PRINT A, F, C, E, D
    50 END
```

(b) Write a program in BASIC to calculate the area under the curve,  $y = x + \frac{1}{\sqrt{x}}$  using the Trapezoidal rule with limit (1, 4) and number of iterations = 20.

(c) Explain Binary Bisection Method.

7. Attempt all parts.

[4 × 3 =

(a) Write a program in Basic to add two  $4 \times 4$  matrix using READ...DATA statement.

(b) (i) Write a program in BASIC to print ASCII code for first character of "COLLEGE".

(ii) What is the full form of CLS. Give its significance.

(c) Write short notes on:

(i) Hybrid Computers

(ii) BASIC