# [This question paper contains 6 printed pages.]

12/5/17

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Your Roll No.....

R No. of Question Paper: 765

G

Unique Paper Code

: 217601

Name of the Paper

: Inorganic Chemistry - V (CHHT-

615)

Name of the Course

: B.Sc. (H) Chemistry

Semester

VI

Duration: 3 Hours

Maximum Marks: 75

## Instructions for Candidates

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

- 2. Attempt any Five questions.
- 3. All questions Carry equal marks.
- 1. (a) Draw the structure of Ferrocene in solid and gaseous state. Why can't Ferrocene be nitrated with HNO<sub>3</sub> directly? How can dinitroferrocene be prepared?
  - (b) Justify the statement "Haem group in the absence of globin chain cannot function as an oxygen carrier".

(c) Give the use of the following reagents (any two) in the identification of ions in qualitative analysis and discuss the chemistry involved.

- (i) Nessler's reagent
- (ii) Sodium bismuthate
- (iii) Potassium thiocyanate
- (d) Inability of a patient's body to synthesize transferrin may lead to anemia as well as overload of iron (siderosis). Do you agree? Justify you answer. Describe the mechanism by which iron is taken up by the cells from transferrin. (3,3,4,5)
- 2. (a) Give reactions to show that Ferrocene resembles thiophen or phenol in its reactivity rather than benzene.
  - (b) Explain the ready reduction of V(CO)<sub>6</sub> to the monoanion.
  - (c) The CO stretching frequency in  $[Fe(CO)_4]^{2-}$ ,  $[Co(CO)_4]^{-}$  and  $Ni(CO)_4$  are 1788 cm<sup>-1</sup>, 1918 cm<sup>-1</sup>, 2121 cm<sup>-1</sup>. Explain.
  - (d) What special features of zinc make it an excellent biocatalyst?
  - (e) Give the chemistry involved in the following tests (any two) of qualitative analysis:

- (i) Chromyl chloride test for Cl- ion
- (ii) Ammonium phosphomolybdate test for PO<sub>4</sub><sup>3-</sup> ion
- (iii) Lime water test for  $CO_3^{2-}$  ion (3,2,3,3,4)
- (a) What are the biochemical effects of exposure to arsenic? Name the antidote for arsenic poisoning.
  - (b) Define organometallic compounds. Which of the following is/are organometallic compound?
    - (i) CH<sub>3</sub>MgBr
    - (ii) Ti(OEt)<sub>4</sub>
  - (c) Why is cisplatin preferred over transplatin as an antitumor drug?
  - (d) Give a systematic procedure for the analysis of an aqueous solution containing only Fe<sup>3+</sup> and Cr<sup>3+</sup> ions. Give the reactions involved. (3,3,4,5)
- 4. (a) What is Chelation therapy? Explain giving two examples.
  - (b) Give the structure of
    - (i) Co<sub>2</sub>(CO)<sub>8</sub> in the solid state

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- (ii) Co<sub>2</sub>(CO)<sub>8</sub> in solution
- (iii) Ni(CO)<sub>4</sub>
- (iv)  $Os_3(CO)_{12}$
- (c) Why does the medium need to be alkaline before passing H<sub>2</sub>S for the analysis of group IV cations?
- (d) What is the importance of the Sodium-potassium pump in the body? Explain its working with illustration. What is the energy source for its working? (3,4,3,5)
- 5. (a) Why is copper an essential element for humans? What are the diseases associated with the excess and deficiency of copper?
  - (b) In qualitative analysis a slight excess of ammonium salts is needed during the precipitation of group V cations, but a large excess is avoided. Explain.
  - (c) Which is more basic towards a proton and why?

    [Mn(CO)<sub>5</sub>]<sup>-</sup> or [Re(CO)<sub>5</sub>]<sup>-</sup>
  - (d) In metal carbonyls, CO forms a bond to the metal through carbon and not though oxygen. Explain with help of MO diagram of CO. Why is CO called a  $\pi$  acid ligand? (4,3,3,5)

6. (a) Ferrocene on reaction with excess of acetic anhydride in presence of AlCl<sub>3</sub>, gives a 1,1' diacetyl derivative as the main product and not the 1,2 derivative. Explain.

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- (b) Describe the tense and relaxed states of Haemoglobin. Explain the change in magnetic behavior of Haemoglobin in going from the "tense" to the "relaxed" state.
- (c) How can you test for NO<sub>3</sub><sup>-</sup> ions in presence of Brions?
- (d) Give the confirmatory tests for the following anions (any three) and give the chemical equations involved
  - (i) BO<sub>3</sub><sup>3-</sup>
  - (ii) C<sub>2</sub>O<sub>4</sub><sup>2-</sup>
  - (iii) S<sub>2</sub>O<sub>3</sub><sup>2-</sup>

(iv)  $F^-$  (3,4,2,6)

- 7. (a) Calculate the member of valence electrons for the following compounds (any four):
  - (i) Fe<sub>3</sub>(CO)<sub>12</sub>
  - (ii) Mn<sub>2</sub>(CO)<sub>10</sub>

- (iii) Co<sub>2</sub>(CO)<sub>8</sub>
- (iv) V(CO)<sub>5</sub>(NO)
- (v) Fe  $(\pi C_5H_5)(CO)$
- (b) Give the classification of elements according to their action in biological systems.
- (c) When conc. sulfuric acid is added to a mixture containing I<sup>-</sup> and Br<sup>-</sup>, I<sub>2</sub> is released followed by Br<sub>2</sub>. Give reason.
- (d) What is the function of the enzyme carbonic anhydrase? Describe the mechanism of action of the enzyme.

(4,4,3,4)

Your Roll No...

Sr. No. of Question Paper: 766

Unique Paper Code : 217603

Name of the Paper : Organic Chemistry V (CHHT-616)

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

Semester : VI

Duration: 3 Hours Maximum Marks: 75

## Instructions for Candidates

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

- 2. Answer six questions in all.
- 3. Question No. 1 is compulsory.
- 1. Answer any five parts:
  - (a) How will you distinguish between cis and trans -cinnamic acid by means of NMR? Give approximate J values also.
  - (b) Nitrobenzene absorbs strongly at 1525 and 1350 Cm<sup>-1</sup>. Assign these peaks to the corresponding vibrational frequencies.

- (c) Which of the two ,o-Benzoquinone and p-Benzoquinone is deeper in colour? Give Reason.
- (d) List the following group of monomers in order of decreasing ability to undergo anionic polymerisation. Give Reason also.

$$CH_2$$
= $CH$ — $CH_3$ ,  $CH_2$ = $CH$ — $Cl$ ,  $CH_2$ = $CH$ -- $CN$ 

(e) Deduce possible monomers for polymers with following repeating units.

(ii) 
$$-(--CO-(CH_2)_6---NH---)_n$$

(f) Which of the following two compounds will give higher λ max value? (No data is required). Give reason for your answer.

(g) In a given organic compound, two kinds of protons show signals at 50 Hz and 200 Hz using a 60 MHz NMR instrument. What would be their equivalent positions using 90 MHz instrument? (3×5)

. (a) Acetylenic protons are more shielded than ethylenic protons. Give the name of the "Effect" and explain this phenomenon.

Describe the splitting pattern of protons "b" and "c" with the help of a diagram. Give J values also. (2)

- (c) Write the structural formulae for the compounds with the following molecular formulae that show only one signal in their NMR spectra.
  - (i)  $C_5H_{12}$  (ii)  $C_3H_6$  (iii)  $C_2H_6O$  (iv)  $C_8H_{18}$  (4×3)
- . (a) Ethylacetate shows carbonyl stretching absorptions at 1735 cm<sup>-1</sup> whereas phenylacetate at 1770 cm<sup>-1</sup>. Explain.
  - (b) A conc. solution of C<sub>2</sub>H<sub>5</sub>OH in CCl<sub>4</sub> as well as one of CH<sub>2</sub>OHCH<sub>2</sub>OH has a broad O-H Stretching frequency near 3350 cm<sup>-1</sup>. On dilution with CCl<sub>4</sub>, the spectrum of CH<sub>2</sub>OHCH<sub>2</sub>OH does not change, but that of C<sub>2</sub>H<sub>5</sub>OH shows a sharp O-H stretch at 3600 cm<sup>-1</sup> in addition to the broad band at 3350 cm<sup>-1</sup>. Explain this observation.

- (c) Calculate the approximate wavenumber of fundamental absorption peak due to the stretching vibrations of N-H bond. Force constant for N-H bond is 6.4×10<sup>5</sup> dynes cm<sup>-1</sup>. Reduced mass 0.933×1.67×10<sup>-24</sup> g. (4×3)
- 4. (a) An  $\alpha$ ,  $\beta$  unsaturated ketone shows following data:

λ max in Hexane 230 nm ε max 12600 329 nm 41 AND

λ max in Water

243 nm ε max 10000 305 nm 60

Assign the various transitions. Explain the shift when the solvent is changed from Hexane to water.

(b) Compounds A, B, and C have the molecular formula  $C_5H_8$ . On hydrogenation all give n- pentane. Their UV shows the following values.

 $\lambda$  max : A, 176; B, 211; C, 215 nm. (1-Pentene has  $\lambda$  max 178 nm)

What are the likely structures for A, B, and C?

(c) Calculate  $\lambda$  max for the following compounds.

Base value for  $\alpha$ ,  $\beta$  unsaturated cyclopentenone -205 nm, cyclohexenone-215

α- Alkyl group / Ring residue 10 nm,

β- Alkyl group / Ring residue 12 nm,

γ, δ etc - Alky group/Ring residue 18 nm,

Exocyclic double bond 5 nm

Homoannular diene system 39 nm,

Double bond extending conjugation, 30 nm. (4×3)

- 5. (a)  $A \xrightarrow{Sn/HCl} 1$  Naphthylamine + 4-Hydroxy-l-naphthylamine. What is A?
  - (b) Explain, why during the synthesis of azo dyes
    - (i) Temperature is kept low (0 −5°C)
    - (ii) A suitable pH is required.
    - (iii) Diazonium compound is coupled with a compound having highly activating group.
  - (c) Give one synthesis of congored. Give its colour change as pH changes. For what kind of fiber, can it be used directly? (2,6,4)
- (a) LDPE is a branched polymer. Give its synthesis and mechanism for formation.

- (b) Differentiate between thermoplastics and thermosets Give one example of each.
- (c) How will you prove that two isatin units have 2:2' linkage in indigotin. (4,2,6)
- 7. An organic compound with molecular formula  $C_{10}H_{12}O_2$  shows
  - (i) UV absorption at 220 nm (E max 1800)
  - (ii) IR spectrum absorption bands are at 3077, 2976, 1745, 1608, 1497, 1456 cm<sup>-1</sup>
  - (iii) In NMR, Signals are as follows:

 $\delta$  7.3 s,

4.3 (t, J=7 Hz)

3.0 (t, J=7 Hz)

2.1 s

in the ratio 2.5:1:1:1.5

Calculate DBE. Explain UV, IR, NMR Data. Give the structure of the compound. (12)

- 8. Write short notes on any three of the following:
  - (a) Novolac Resin
  - (b) Biodegradable polymers with one example
  - (c) Crystal violet
  - (d) Malachite green

 $(4\times3)$ 

(2200)

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Your Roll No.....

No. of Question Paper: 767

G

Unique Paper Code

217605

Name of the Paper

: Physical Chemistry – V [CHHT 617]

Name of the Course

B.Sc. (Honours) Chemistry

Semester

VI

Duration: 3 Hours

Maximum Marks: 75

### Instructions for Candidates

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

- 2. Total Six questions to be answered.
- 3. Question No. 1 is compulsory.
- 4. Answer any FIVE other questions.
- 5. Use of scientific calculator is allowed but it cannot be shared. Logarithmic tables may be provided if required.
- 6. PHYSICAL CONSTANTS:

Planck's constant  $6.626 \times 10^{-34}$  Js

Velocity of light  $3 \times 10^8 \text{ ms}^{-1}$ 

Avogadro's number  $6.023 \times 10^{23} \text{ mol}^{-1}$ 

Nuclear magneton  $5.051 \times 10^{-27} \, \text{JT}^{-1}$ 

Bohr magneton  $9.274 \times 10^{-31} \text{ JT}^{-1}$ 

Mass of electron  $9.109 \times 10^{-31}$  kg

1 atomic mass unit  $1.66 \times 10^{-27} \text{ kg}$ 

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#### 1. Attempt any FIVE:

(a) Arrange the following in order of descending energy:  $10 \text{ cm}^{-1}$ ,  $1 \times 10^{-23} \text{ J}$ , 0.01 m, 1 MHz.

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- (b) Show that the operators  $\hat{L}^2$  and  $\hat{L}_z$  commute. What inference can be drawn from this property?
- (c) Draw an energy level diagram to explain the phenomena of fluorescence and phosphorescence.
- (d) (i) Write the expression for the Schrodinger's equation for a particle of mass m existing in a onedimensional box of length L.
  - (ii) What are the units, if any, of the wavefunction for this system?
- (e) Represent diagrammatically the relation between the Cartesian coordinates and the spherical coordinates and give their mathematical expressions.
- (f) The rotational spectrum of <sup>127</sup>I<sup>35</sup>Cl consists of lines equally spaced by 0.114 cm<sup>-1</sup>. Calculate the bond distance for iodine monochloride. (3×5=15)

 (a) Evaluate the mean value of the radius (r) at which the electron in the H-atom is found, given that

$$\psi_{2,0,0} = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{\frac{3}{2}} \left(2 - \frac{r}{a_0}\right) \exp\left(-\frac{r}{2a_0}\right)$$

where ao is the Bohr radius.

$$\left[\int_{0}^{\infty} x^{n} \exp(-ax) dx = \frac{n!}{a^{(n+1)}}\right]$$

- (b) Will this value of  $\langle r \rangle$  be the same for Li<sup>2+</sup>? Explain briefly.
- (c) Draw the energy level diagram for Ne<sub>2</sub> and show that this molecule cannot exist. (5,2,5)
- (a) Write the complete valence bond wavefunctions for hydrogen molecule.
  - (b) Explain the following terms briefly: fundamental absorptions, overtones and hot bands.

(c) An unnormalized wavefunction of an electron in a carbon 5. nanotube of length L is  $\sin\frac{2\pi x}{L}$ . What is the probability of finding the electron between x=0 to x=L/2.

$$\left[\int_{0}^{L} \sin^{2} ax \, dx = \int_{0}^{L} \frac{1}{2} \left(1 - \cos \frac{2ax}{L}\right) dx\right]$$
 (4,4,4)

- 4. (a) Write the Hamiltonian for Helium atom and setup the corresponding Schrödinger equation.
  - (b) A strong absorption band is observed for <sup>12</sup>C<sup>16</sup>O in the IR region at 2170 cm<sup>-1</sup>. Assuming harmonic potential, calculate
    - (i) Vibrational frequency in Hz
    - (ii) Vibrational time period in s
    - (iii) Zero point energy in J.
  - (c) The bond length of  ${}^{1}H^{19}F$  is  $91.68 \times 10^{-12}$  m. Where does the axis of rotation intersect the molecular axis? (4,4,4)

(a) What is the selection rule for Raman rotational spectrum of diatomic molecules? Show that the Raman lines will appear at wavenumbers given by

$$\overline{\nu}=\overline{\nu}_0\pm 4B\bigg(J+\frac{3}{2}\bigg)\quad where\quad \overline{\nu}_0\quad is\ the\ wavenumber$$
 corresponding to the Rayleigh Line.

(b) Derive the following:

$$v_{max} = \frac{1}{2x_e} - \frac{1}{2}$$
 where the symbols have their usual meaning.

- (c) A solution shows a transmittance of 20% when kept in a cell of 2.5 cm thickness. Calculate the concentration of the solution given that the molar absorption coefficient has a value of 12 × 10<sup>3</sup> dm<sup>3</sup> mol<sup>-1</sup> cm<sup>-1</sup>. (4,4,4)
- 6. (a) State the Variation Theorem.
  - (b) Identify the following molecule and assign frequencies to the possible modes of vibrations. Justify the assignment of the frequencies and suggest a possible structure for the molecule.

Molecular Formula	Electronic Configuration	Transition Frequency (cm <sup>-1</sup> )	IR	Raman
AB <sub>2</sub>	A: 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup> B: 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup>	1330		Active
		2349	PR contour	
	B: 1s-2s-2p	667.3	PQR contour	

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- (c) The ESR spectrum of atomic hydrogen is recorded on a spectrometer operating at 9.302 GHz. At what magnetic field does resonance occur? ( $g_e = 2.0023$ ) (3,6,3)
- 7. (a) Indicate which of the following will lead to an eigenvalue equation. Report the eigenvalue, if any
  - (i)  $\frac{d}{dt} \exp(i\omega t)$

(ii) 
$$\left(\frac{d^2}{dx^2} + 2\frac{d}{dx} + 3\right) \exp(\alpha x)$$

(b) In the MO treatment for hydrogen molecule ion the LCAO-MO wavefunction is  $\psi_{MO} = c_1 \phi_{H_a} + c_2 \phi_{H_b}$  where 9.  $\phi_{H_a}$  and  $\phi_{H_b}$  correspond to the normalized 1s wavefunctions for the hydrogen atoms  $H_a$  and  $H_b$  in the ion.

- (i) Write the expression for the Hamiltonian.
- (ii) Optimize the energy with respect to c<sub>1</sub> and c<sub>2</sub> and express the result in the form of secular determinant.
- (iii) Expand the determinant and evaluate the energy for the bonding molecular orbital.
- (c) Define Hermitian operator and give an example. (3,6,3)
- (a) Sketch the low and high resolution NMR spectra of CH<sub>3</sub>COOCH<sub>2</sub>CH<sub>3</sub> (ethyl ethanoate) and CH<sub>3</sub>CH<sub>2</sub>COOCH<sub>3</sub> (methyl propanoate). Explain the differences briefly.
- (b) Sketch the ESR spectrum of benzene radical anion.
- (c) Butadiene is more stable than two molecules of ethene.

  Explain this on the basis of Huckel Molecular Orbital
  Theory. (5,3,4)

Write short notes on any three:

(a) Heisenberg Uncertainty Principle

- (b) Effect of isotopic substitution on rotational spectra
- (c) Larmor Precessional Frequency
- (d) Free Electron Molecular Orbital Model (3XY)(3

[This question paper contains 8 printed pages]

Your **Rø**ll No. : .....

Sl. No. of Q. Paper : 768 G

Unique Paper Code : 217607

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

Name of the Paper : Applications of

Computer in Chemistry

Semester : VI

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 in **all**. Question **NO.1** is compulsory.

(c) All questions carry equal marks.

1. (a) Write the following expressions in BASIC 3×5

(i) B=D 
$$(1+R)^n log_{10}(X)$$

(ii) 
$$a = \frac{27R^2T^2}{64P}$$

(iii) 
$$D(f) = 4\pi c^2 \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{\left(-\frac{mc^2}{2kT}\right)}$$

(b) What is the purpose of the following LIBRARY FUNCITONS?

(i) ABS(X)

(ii) ATN(X)

(iii) INT(X)

(c) Identify the invalid variables and write the correct ones also identifying type (numeric or alphanumeric):

(i) 1A

(ii) 2S\$

(iii) \$N

(d) Identify the invalid constants. Write the correct form and identify their type (numeric of string):

(i) 12E10<sup>2</sup>

(ii) '1212'

(iii) 'NAME'

(e) Define the following terms:

(i) RAM

(ii) ASCII

(iii) Byte

2. (a) Identify & correct the error in the following BASIC statements:

(i) LET N1="25.5"

(ii) DATA, 7+2, 13,"NAME", SWEET

(b) Distinguish between:

(i) Interpreter and Compiler

(ii) Software and Hardware

2

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(c) Write a program in BASIC (using user-defined functions) for finding the roots of the following polynomial equation using Newton Raphson Method within the tolerance 10<sup>-6</sup>:

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

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(d) Write a program to calculate the pressure exerted by 2 moles of ammonia gas enclosed in a vessel of 5 L capacity at 27° C for ideal gas equation (PV=n RT) and van der Waals equation (P=RT/V-b)-a/V^2). Given that for ammonia: a=4.17 atm L² mol-1 and b=0.046 L mol-1, Gas constant R=0.0821 dm³ atm k-1 mol-1:

3. (a) What is displayed on the output screen when the following segment of the code is executed?

200 DIM A(2,3)

210 FOR I=1 TO 2

220 FOR J=1 TO 3

230 LET A(I,J)=I+J

240 NEXT J

250 NEXT I

260 PRINT A (1,2); A(2,1); A(2,2)

3

2

P.T.O.

(ˈp)	Rewrite the following programs THEN-ELSE commands:	using	IF.
	10 FOR I = 1 TO 100		
	20 READ N\$, S1,S2		
	30  LET S = S1+S2		
•	40 PRINT N\$, S		
	50 NEXT I		
9	60 DATA,, etc.		
	70 END		

(c) Write the BASIC statement to produce the following effects:

- (i) Assign a string 34 to a variable
- (ii) Bring the pointer back to the first value in the data block created by the program
- (iii) Truncate X and return the integer part
- (iv) To draw four concentric circles 4
- (d) Comment on the errors in the following program 'to find the factorial of a number' and correct them:

```
10 CLSS
```

20 INPUT"ENTER THE NUMBER"N=5

30 F=1

40 WHILE N>=0

50 F=F X N

60 N=N-1

70 WIND

80 PRINT FACTORIAL =F

90 STOP

-

**4.** (a) Draw the output and show the position of the coordinates for the following set of statements:

10 CLS

20 SCREEN 1

30 VIEW (10,10)-(300,180),,1

40 WINDOW (0,0)-(50,50)

50 LINE (1,1)-(25,1)

50 END

1

(b) Let A=1 and B=2. Are the following conditions true or false?

(i) ((2\*A+6)>(B+1) AND (INT(B/3)=1)

(ii) NOT (A\*B<>1)

- (c) Comment on the errors in the following program and correct them:

  REM TO DRAW A CIRCLE IN GRAPHICS SCREEN 2

  SCREEN VIEW (X,Y)-(300,180)

  CIRCLE 20,,(150,150)

  LOCATE (20): PRINT "CIRCLE# END
- (d) WAP in BASIC to plot molar conductance  $\Lambda_m vs\sqrt{c}$ . Fit the data to a straight line using equation

 $\Lambda_{\rm m} = \Lambda_{\rm m}^0 - k\sqrt{c}$  and calculate  $\Lambda_{\rm m}^0$ .

Conc./M	Molar conductance/S m <sup>2</sup> mol <sup>-1</sup>
17.68	42.45
10.8	45.91
2.67	51.81
1.28	54.09
0.83	55.78
0.19	57.42

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

intercept= 
$$(\sum x_i^2 \sum y_i - \sum x_i y_i \sum x_i)/(N \sum x_i^2 - (\sum x_i)^2)$$

- 5. (a) Using DIM statement, explain the difference between 1-D array and 2-D array. 2
  - (b) If A\$="TO ERR IS HUMAN"

    B\$="TO FORGIVE, DIVINE"

    Then find the values of:

(i)RIGHT\$ (B\$,2)

(ii)A\$+ "" +B\$

(c) Write a program to evaluate the following series:

(i) 
$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots$$

(d) Using the standard rule of matrix multiplication, write a program to calculate the product of two matrices A and B

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad B = \begin{bmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \\ 2 & 2 & 2 \end{bmatrix}$$

6. (a) What is displayed when the following code is run?

200	DEF FNF $(X)=3*X+1$		
210	DEF FNG $(X,Y)=X^2+Y^2$		
220	LET Z=2	- 11	
230	PRINT FNF $(Z)$ ; FNG $(Z+1,Z)$	5-1)	0
240	PRINT FNF (FNG(1,2))		2
1 <del>25</del> .01275	7	P.T.	O.

- (b) With the help of suitable examples, explain the meaning of the following error massages:
  - (i) Subscript out of range
  - (ii) Type Mismatch

2

(c) Write a program (using subscripted variables) to estimate the mean, variance and standard deviation of a set of N numbers. Provide the data using INPUT statement.

$$Mean = \frac{1}{n} \sum_{i=1}^{n} x_{i}$$

Variance = 
$$\frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x})^2$$

Standard Deviation =  $\sqrt{\text{Variance}}$ 

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(d) Write a program in BASIC to find the value of the integral using trapezoidal rule with n=6.

$$\int_0^1 dt / \sqrt{(t^2 + 1)(3t^2 + 4)}$$



S.No. of the Question Paper:

1660

Roll No.

Unique Paper code

: 2171602 Theory Physical: Quantum chemistry, Photochemistr : Physical Chemistry, Paner XVI and Surface Chemist

Name of the Paper

: Physical Chemistry, Paper XVI

Name of the Course

: B.Sc (Honours) Chemistry

Semester

: VI

Duration

: 3 Hours

Maximum marks

: 75

#### Instructions for Candidates

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

Attempt only six questions out of eight. Question No. 1 is compulsory.

Use of scientific calculator and Logarithmic tables is allowed.

Attempt all parts of a question together.

#### Physical Constants

Planck 's constant

 $6.626 \times 10^{-34} \text{ J s}$ 

Velocity of Light

 $3 \times 10^{8} \text{ m s}^{-1}$ 

Avogadro's Number

 $6.022 \times 10^{23} \text{ mol}^{-1}$ 

Mass of Electron

 $9.1 \times 10^{-31} \text{ kg}$ 

Boltzmann Constant

 $1.38 \times 10^{-23} \text{ J K}^{-1}$ 

### Attempt any five:

- Show that  $e^{\alpha x}$  is an Eigen function of the operator  $\frac{d^n}{dx^n}$ . What is the Eigen value? (a) Differentiate between Eigen value and expectation value.
- Write down the Hamiltonian operators for Li atom and He atom. Explain the Born-(b) Oppenheimer approximation while constructing it.
- Why the quantum number 'n' cannot be assigned a zero value while solving for the (c) particle in a 1-D box? Give the units of  $\psi^2$  for a particle in a 1-D box.
- Why is 1s orbital of one atom combined linearly with only two of the three 2p orbitals of another atom while constructing molecular orbital using LCAO-MO approach?
- Photosynthesis is a photosensitized reaction. Explain. (e)

- (f) Substances like charcoal or silica gel are used to create very high vacuum. Explain. Why can't physisorption be observed at a temperature much above the critical temperature of adsorbate?
- (g) Explain why only exothermic chemisorption is spontaneous.

3 x 5

- 2. (a) Calculate the expectation value of linear momentum, p and its square, p<sup>2</sup> for a particle in a 1-D box of length *l*. Give their physical significance.
  - (b) Determine the value of x at which the ground state wave function of the harmonic oscillator exhibits the maximum.

    Given:  $\psi_0 = (\alpha/\pi)^{1/4} \exp(-\alpha x^2/2)$
  - (c) Calculate the (i) average distance (expectation value) and (ii) the most probable distance of the electron from the nucleus in the ground state of the Hydrogen atom.

Given: 
$$R_{1s} = 2\left(\frac{1}{a_o}\right)^{3/2} exp\left(\frac{-r}{a_o}\right)$$
 and  $\int_0^\infty x^n \exp(-ax) dx = \frac{n!}{a^{n+1}}$ 

4,4,4

- (a) Discuss the need of approximate methods for determining the solution of Schrodinger equation for multi-electron atoms. State and explain the Variation theorem.
  - (b) Make use of this theorem to calculate the average ground state energy of the H atom using the trial wave function:  $\psi = \exp(-\alpha x)$ .

    Given: The Hamilotonian operator for the ground state energy of Hydrogen is given by  $\hat{H} = \frac{-h^2}{2\mu r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) \left( \frac{e^2}{(4\pi\epsilon_0)r} \right)$   $\int_0^\infty x^n \exp(-ax) \, dx = \frac{n!}{a^{n+1}}$
  - (c) Using LCAO-MO treatment for the H<sub>2</sub><sup>+</sup>, prove that the energy of the bonding MO is less than the energy of the anti-bonding MO.

4,4,4

- 4. (a) Naphthalene may be considered to be a rectangular box of length and breadth equal to 0.8 nm and 0.4 nm, respectively. Calculate the expected wave number of radiation required to give the first excited state.
  - (b) What is an acceptable wave function? Giving reasons, state which of the following wave functions are acceptable over the range  $0 \le x \le 2\pi$

(i)  $\sin x$  (ii)  $\tan x$  (iii)  $\cos x + \sin x$ 

(c) Find the commutator for the operators  $x^2$  and  $d^2/dx^2$ .

4,4,4

- 5. (a) Using LCAO-MO approach, draw the shapes of Molecular Orbitals involved in bonding of H<sub>2</sub>O molecule and construct the Molecular Orbital energy level diagram for H<sub>2</sub>O molecule.
  - (b) State the physical significance of S (overlap integral), J (coulomb integral) and K (resonance/exchange integral) in Valence bond theory.
  - (c) Explain the magnetic behaviour of the following on the basis of Molecular orbital approach: NO, NO, NO and N<sub>2</sub>

4,4,4

- 6. (a) Give the postulates of and derive the expression for the Langmuir adsorption isotherm. What are the limiting cases?
  - (b) Explain different types of adsorption isotherms on the basis of BET equation.
  - (c) The volume  $\nu$  of nitrogen adsorbed per gram of active carbon at 0°C at a series of pressure P are given as follows:

<i>P</i> / Pa	500	2000	3000	4500	7500
FIRa	300	2000	562	7.01	10.33
$v / cm^{3} g^{-1}$	0.943	3.48	5.00	7.01	10.33

Plot the data according to the Langmuir isotherm and determine K,  $\nu$  and  $\theta$  at 4500 Pa.

4.4.4

- 7. (a) State the Einstein's Law of photochemical equivalence. Write the expression of Quantum yield and explain with example.
  - (b) Give at least two reasons each for low and high quantum yield.
  - (c) The photochemical decomposition of HI is given as:

$$2HI \rightarrow H_2 + I_2$$

The mechanism is given as:

HI + hv 
$$\xrightarrow{l_{abs}}$$
 H + I

H + HI  $\xrightarrow{k_2}$  H<sub>2</sub> + I

I + I  $\xrightarrow{k_3}$  I<sub>2</sub>

H + I<sub>2</sub>  $\xrightarrow{k_4}$  HI + I

Derive the expression for the quantum efficiency of the overall reaction.

4,4,4

- 8. Write short notes on any three:
  - (a) HMO treatment of Ethene
  - (b) Chemical Actinometry
  - (c) Photostationary states
  - (d) Gibbs Adsorption Isotherm
  - (e) Surface Area determination for monolayer formation

4,4,4

St. No. 17 G.P 1661

Unique Paper Code

Name of the Paper :

Name of the Course :

SETTIFICATION

Direction

Max.mum Marks

Inorganic+ Physical (Paper No. 17)

B.Sc. (H) Chemistry

VI

3 hours

75



#### Instructions for Candidates

The question paper carries two sections (Section A and B). Each section carries 37 1/2 marks.

#### Use separate sheet for each section

#### Section A

Attempt any three questions in all. Question No. 1 is compulsory and carries 7 1/2 marks.

1. Answer the following:

a) Why Zinc Sulphide is used in luminescent devices?

b) Why nanomaterials are different from bulk materials?

c) What is Quantum Confinement?

Why solids exhibiting anionic mobility are rarer than cationic conductors?

d) What are topotactic reactions?

e) What is the origin of colour in the following inorganic pigments

(i)CoAl2O4

(ii)PbCrO<sub>4</sub>

f) Define the terms: Static self-assembly and Dynamic self-assembly

[1,1,1,1,1 1/2,2]

- 2. a) Write down the steps involved in the preparation of silver metallic nanoparticles.
  - b) At T=0, no one dimensional solid is a metal. Comment.
  - c) What is One-dimensional control in carbon nanotubes? How can you prepare SWNTs and MWNTs using arc discharge method?

d) Describe ion exchange method for preparation of inorganic solid materials

(4, 3, 5, 3)

- 3 (a) Compare the chemistry of graphite and C60 in the compounds associated with alkali metal ions.
  - (b) What are the advantages of inorganic pigments?
- (c) Discuss sol gel method for preparation of nanomaterials. Why is it preferred over conventional heat and heat methods?
- (d) Devices made from nanowires have several advantages over those made by photolithography. Explain.

(3, 3, 6, 3)

- Q4: Write short notes on any three of the following:
  - (1)Bionanocomposites
  - (2)Inorganic nanowires
  - (3) Natural and Artficial nanomaterials
  - (4)Intercalation method for synthesis of Inorganic solids
  - (5) Hydrothermal method.

[5x3]

#### Section B

Use of scientific non -programmable calculators is allowed.

Constants: Planck's constant  $h = 6.626 \times 10^{-34} \text{ Js}$ ; Boltzmann constant  $k = 1.38 \times 10^{-23} \text{ JK}^{-1}$ 

Velocity of light,  $c = 3 \times 10^{10}$  cm/s; mass of electron = 9.1 x 10<sup>-31</sup> kg

All questions carry equal marks

#### Attempt any 3 questions:

- 1. (a) H<sub>2</sub> does not give a rotational spectrum whereas HF does. Comment (2)
  - (b) Discuss in brief, the factors responsible for the intensity of microwave (rotational) spectral lines. (2 ½)
  - (c) The rotational spectrum of  $^{79}$ Br $^{19}$ F shows a series of equidistant lines 0.714 cm $^{-1}$  apart. Calculate the rotational constant B, and hence the moment of Inertia and bond length of the molecule. Take the relative atomic weights of  $^{79}$ Br and  $^{19}$ F to be respectively 79 and 19 and absolute mass of H atom = 1.67 x 10 $^{-27}$  kg. (4)

(d) Show that the equation for the quantum number of the level having highest population  $(J_{max})$  is given by

 $J_{max} = \sqrt{\frac{kT}{2Bhc}} - \frac{1}{2}$  where **k** is Boltzmann constant, h is Planck's constant, c is velocity of light and T is the temperature. (4)

#### 2 (a) What are Hot bands?

(b) Roughly sketch the fundamental vibrations of CO<sub>2</sub> molecule and show which of them are Infra-red active and why? (2 ½)

- (c) The spectrum of  ${}^{1}H^{35}Cl$  gas shows a very intense absorption at 2886 cm $^{-1}$ , a weaker one at 5668 cm $^{-1}$  and very weak one at 8347 cm $^{-1}$  at 300K. Calculate vibration frequency (in cm $^{-1}$ ) and zero-point energy (in cm $^{-1}$ ) and force constant of HCl gas. (given that reduced mass ( $\mu$ ) of HCl = 1.62 x 10  $^{-27}$  kg).
- (d) Derive the expression for maximum vibrational quantum number and the maximum value of vibrational energy possessed by an anharmonic oscillator. (4)
- 3. (a) What is Raman effect? Explain the origin of Stokes and anti-Stokes lines. (2)
  - (b) Which of the following molecules are Raman active and why? N<sub>2</sub>, HF, CHCl<sub>3</sub>, H<sub>2</sub>O?

    (2 ½)

(c) A molecule AB2 shows IR and Raman spectra as tabulated below:

$\bar{\nu}$ / cm <sup>-1</sup>	IR	Raman
589	Strong (PQR contour)	Kaman
1285	Very strong (PR contour)	Very strong polo-i-
2224	Very strong (PR contour)	Very strong, polarized Strong, depolarized

Predict the shape of the molecule and assign the various observed lines to the appropriate normal modes of vibrations. (4)

(d) Explain the phenomena of fluorescence and phosphorescence using suitable diagrams.

- 4. (a) State and explain the Frank Condon principle using suitable diagram.<sup>5</sup> (2)
  - (b) Explain the phenomenon of predissociation with the help of a diagram. (2 ½)
  - (c) Consider the free electron molecular orbital description of the linear conjugated molecule octatetraene:

$$CH_2 = CH - CH = CH - CH = CH - CH = CH_2$$
What is the minimum excitation

What is the minimum excitation energy given that C-C bond length is 154 pm

And C = C bond length is 135 pm.

(4)

(4)

(d)	Show that the separation between the maxima in P and R branches of a vibration
	ntion spectrum of a hetero nuclear diatomic molecule is given by

 $\sqrt{\frac{8kTE}{hc}}$ 

where k is the Boltzmann constant, h is Planck's constant, B is the rotational constant. T is the temperature and c is the velocity of light.

St NO 079. P: 1662 : 2171604

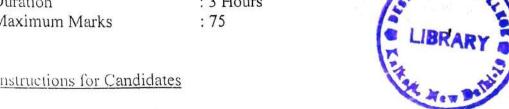
Unique Paper Code

: Organic Chemistry: Chemistry of Biomolecules Name of the Paper

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

Semester : VI

Duration : 3 Hours Maximum Marks



=-8

#### Instructions for Candidates

- 1. Question No. 1 is compulsory.
- 2. Attempt any other five questions.
- What would be the overall yield of a peptide containing 15 amino acid 1 (a) residues if the yield for incorporation of each were 80%?
  - Define Saponification value of an oil. Write the formula for calculating the (b) saponification value experimentally.
  - Draw the structure of a nucleotide of DNA molecule containing Guanine as (c) the base.
  - 2 What is a Coenzyme? Explain briefly giving an example. (d)
  - How is pyruvate converted to lactate under limiting amount of oxygen? (e) 2 Name the enzyme and give the reaction involved.
  - Draw the structure of Glucocerebroside. (1)
  - Draw all possible Zwitter ion structures of Aspartic acid. Which is the actual (g) structure at its pI? Justify the choice of the structure at its pI.
  - Give all the theoretically possible tautomeric forms of base Thymine. Out of 2. (a) these, which form is present in DNA? Give the Wheeler and Liddle method of synthesis of Thymine.
    - Write the structures showing specific hydrogen bonding between following (b) pairs of bases in nucleotides.
      - (i) Uracil and Adenine
      - (ii) Cytosine and Guanine
    - Draw the structures of glyceryl tristearate and glyceryl trioleate. Explain (c) which has a higher melting point. Calculate the iodine value of glyceryl trioleate.
  - Outline the steps involved in the synthesis of a tripeptide Phe-Leu-Ala by (a) 3. Merrifield automated solid phase peptide synthesis.
    - Explain the reactions involved in identifying the N-terminal amino acid of a (b) tripeptide Gly-Ala-Val by Sanger's method. What is the disadvantage of this method as compared to Edman's method for N-terminal analysis of peptides or proteins.

4.	(a) (b)	Discuss briefly the various steps involved in the Kreb's cycle.  Differentiate between reversible and irreversible inhibitors giving suitable	6
	<i>t</i> ×	examples.	3
	(c)	What are essential fatty acids. Give two examples along with their structure	res.
5.	(a)	Outline the synthesis of Phenylalanine starting from glycine using Erlenmeyer azlactone synthesis.	4
	(b)	ATP is called the universal currency of cellular energy. Explain giving its hydrolytic pathway.	4
	(c)	The acid component of a Cholesterol ester is a fatty acid such as oleic acid. Draw the structure of oleic acid and its Cholesterol ester.	4
6.	(a)	One of the strands of DNA molecule shows nucleotide base sequence as 5'- A-T-G-A-C-C-A-T-G-C-A-A-3'. Write down the sequence of bases or complimentary DNA strand and transcripted messenger RNA strand, given the name of bases also set to 5' and the name of bases also set to 5'.	n vin <sub>i</sub>
	(b)	the name of base closest to 5' end in each case.  A nonapeptide has the molecular formula Arg <sub>2</sub> ,Gly <sub>1</sub> ,Phe <sub>2</sub> ,Pro <sub>3</sub> ,Ser <sub>1</sub> . The of 2,4- Dinitroflurobenzene and Carboxypeptidase shows that both term residues are arginine. Partial acid hydrolysis of the nonapeptide gives the following fragments  Phe.Ser + Pro.Gly.Phe + Pro.Pro + Ser.Pro.Phe + Phe.Arg + Arg.Pro	use una
	(c)	What is the amino acid sequence of the nonapeptide?  Name the amino acid triad responsible for the enzymatic activity of tryp Discuss the mechanism of action of trypsin.	4 osin 4
7.	(a)	Give the reaction pathway of conversion of glycerol to glyceraldehyde 3-	
	(b)	phosphate after it is obtained during catabolism of fats.  Draw the Fischer projection formulae of all the possible stereoisomers amino acid Threonine, give their names and label them as D or L. Indicate relationship between these stereoisomers.	3 S O
	(c)	the relationship between these stereoisomers.  An elemental analysis of Cytochrome c, an enzyme involved in oxidati reduction processes, gave 0.43% Fe and 1.48 % S. What is the minimum number of iron at per molecular weight of the enzyme? What is the minimum number of sulphur atoms molecule of enzyme? (Atomic weight of Fe = 55.8 and S = 32)	6 ion nun
8.		Write short notes on the following (any three):	
		<ul> <li>(i) Transcription</li> <li>(ii) Rancidity of oils and fats</li> <li>(iii) Watson and Crick Model of DNA</li> <li>(iv) Electrophoresis</li> </ul>	
		(v) Liposomes and their biomedical applications 3×4	- 6