(iii) Using Molecular Orbital theory, construct the total wavefunction for H_2 molecule. What does each term represent? (5)

[This question paper contains 12 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 7028 **K**

Unique Paper Code : 2172524701

Name of the Paper : Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Elements of Quantum Chemistry

Name of the Course : **B.Sc. (Prog.) Life Sciences**

Semester : VII

Duration : 3 Hours Maximum Marks : 90

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. There are **three** sections in this paper; **Section A:** Inorganic Chemistry, **Section B:** Organic Chemistry and **Section C:** Physical Chemistry.
3. Each section has **three** questions out of which attempt any **two** in each section.
4. Use separate answer-sheets for each section.

P.T.O.

Section A: Inorganic Chemistry

1. Describe the following with suitable examples :

   (a) Catalytic properties of d block elements

   (b) Magnetic properties of lanthanides.

   (c) Frost diagram (5,5,5)

2. (a) Given below is the Latimer diagram for Fe in acidic medium :

$$FeO_4^{2-} \xrightarrow{2.20} Fe^{3+} \xrightarrow{0.77} Fe^{2+} \xrightarrow{-0.47} Fe$$

   Answer the following questions :

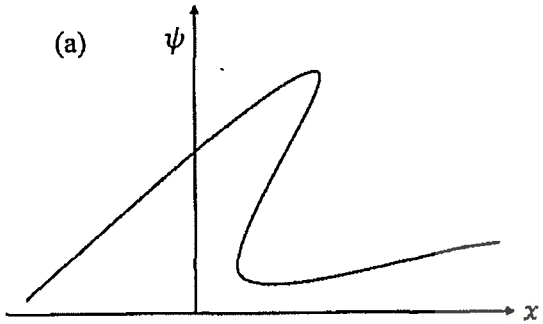
   (i) Is there any tendency of Fe^{2+} to reduce to Fe? Give reasons.

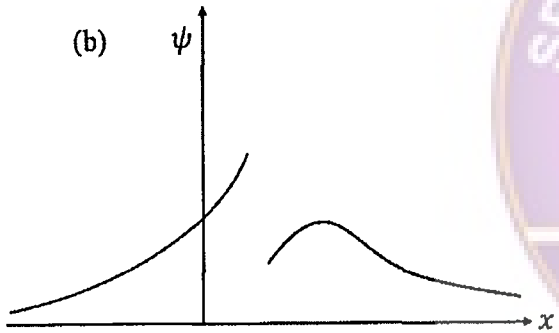
   (ii) Write half reaction for the conversion of FeO_4^{2-} to Fe^{3+}.

   (b) $\hat{A} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ and $\hat{B} = x$

3. (i) A diatomic molecule AB undergoes vibrational motion according to the harmonic oscillator model. Write the mathematical expression for the Hamiltonian, Schrödinger equation and the vibrational energy expression for this system. What will be the zero point energy? (5)

   (ii) Show that $\psi = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$ is an eigen function to the kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ and hence determine the value of kinetic energy. (5)





(iii) Determine whether operators $\hat{A}$ and $\hat{B}$ commute if: (5)

(a) $\hat{A} = 3x^2$ and $\hat{B} = \frac{\partial}{\partial x}$

(iii) Is there any state which undergoes disproportionation? Explain

(iv) Calculate E° for Fe^{3+} / Fe change.

(v) Why is FeO_4^{2-} a strong oxidizing agent?

(b) Give their configuration and predict which of the following will be coloured in aqueous solution?

Ti^{3+}, V^{3+}, Sc^{3+}, Mn^{2+}, Fe^{3+}

(c) What are lanthanides? Explain lanthanide contraction and its consequences. (5,5,5)

3. (a) Why do some lanthanides exhibit unusual oxidation states. Explain.

(b) Discuss the tendency of transition elements to form complex compounds.

(c) Distinguish between transition elements and inner transition elements for any five properties. (5,5,5)

Section B: Organic Chemistry

1. (a) Elucidate the structure of organic compound with molecular formula $C_6H_5NCl_2$, the NMR spectrum of the compound is shown below. The normal carbon -13 and DEPT experiment result are tabulated. The infrared spectrum shows peaks at 3432 and 3313 cm^{-1} and a series of medium sized peaks between 1618 and 1466 cm^{-1}. (10)

Normal Carbon -13 Ppm	DEPT-135	DEPT- 90
118	Positive	Positive
119.5	No Peak	No Peak
128	Positive	Positive
140	No Peak	No Peak

(iii) Draw the radial wavefunction plots and the radial distribution function plots for the electron in 2s and 2p orbitals of the hydrogen atom. Determine the number of radial nodes in each case. (5)

2. (i) Why is n = 0 not permitted for a particle in a one-dimensional box, whereas v = 0 is permitted for a diatomic molecule undergoing harmonic oscillations? (5)

(ii) Define well-behaved wavefunctions. State whether the following functions are well-behaved or not. Give reason for your answer. (5)

(b) Write short note on any **two** of the following : (2.5,2.5)

(i) NOE signal enhancement

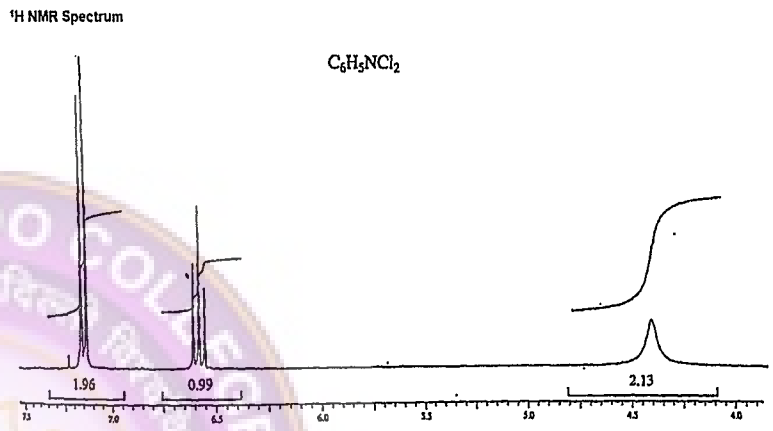
(ii) Nitrogen rule in Mass Spectrometry

(iii) Rule of 13 in Mass Spectrometry

Section C: Physical Chemistry

1. (i) Write the Schrödinger equation and the total energy expression for a particle of mass m confined in a three-dimensional box of lengths a, b and c along the x, y and z axes, respectively. What is degeneracy? (5)

(ii) Determine the normalization constant A for the wavefunction $\psi = A \sin\left(\frac{n\pi x}{a}\right)$ defined in the region $0 \leq x \leq a$ and for which n is an integer. (5)



(b) Discuss any **two** questions. (5)

(i) Write notes on K-band and R-band.

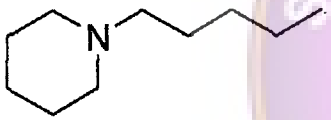
(ii) Why is methanol a good solvent for UV but not for IR determination?

(iii) Explain why absorption bands are formed in ultra-violet spectrum instead of sharp peaks?

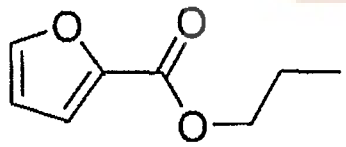
P.T.O.

2. (a) Identify the site of initial ionization under EI conditions, determine the structure of the ion indicated by the m/z values and draw a fragmentation mechanism that accounts for the formation of the following fragment ions : (10)

(i) The Fragment ion at m/z = 98 (base peak in spectrum)



(ii) The Fragment ion at m/z = 95 (base peak in spectrum)



(b) Predict the structural formula for the compounds (any two) with the following molecular formulae showing only one PMR signal each. (5)

(i) C_8H_{18}

(ii) C_2H_6O

(iii) C_5H_{12}

3. (a) Elucidate the structure of organic compound, the ^1H NMR spectrum of compound has 3H triplet at 1.4 ppm, 2H quadrat at 4.2 ppm, 2H triplet at 3.6 ppm, 2H triplet at 3.4 ppm. The mass spectrum shows m/z: 180 (10%), 182 (10%), 136 (100%), 138 (100%). The infrared spectrum shows peak at 1724 cm^{-1}. (10)