Q.P. Code : 35105

[Time: 2½ Hours] **[Marks: 60]**

Please check whether you have received the right question paper.

N.B:
1. All questions are compulsory.
2. Figures to the right indicate full marks.
3. Use of non-programmable scientific calculator is allowed.

Useful constants:-

$c = 2.998 \times 10^{8}\ ms^{-1}$
$R = 8.314\ JK^{-1}\ mol^{-1}$
$h = 6.625 \times 10^{-34}\ Js$
$m_e = 9.110 \times 10^{-31}\ kg$
$N_A = 6.022 \times 10^{23}\ mol^{-1}$
$e = 1.602 \times 10^{-19}\ C$
$k = 1.3811 \times 10^{-23}\ JK^{-1}$
$1\ J = 6.24 \times 10^{18}\ eV$
$1\ eV = 8.06 \times 10^{3}\ cm^{-1}$
$1\ amu = 1.66 \times 10^{-27}\ kg$
C = 12, O = 16

1. (a) Attempt **any two** of the following:-

(i) What are the conditions for a wave function to be acceptable? A wave function is given as $\psi = \cos x$ **04**
Is it acceptable?
Is it normalized? Explain

(ii) For the Hermite's differential equation **04**

$$\frac{d^2F}{dy^2} - 2y\frac{dF}{dy} + \left(\frac{\propto}{\beta} - 1\right)F = 0$$

Obtain the recursion formula

(iii) State the main postulates of quantum mechanics. **04**

(iv) The particle in a one dimensional box of length L has the wave function **04**

$$\psi_n = A\sin\frac{n\pi x}{L}$$

Find the normalization factor A in the range zero to L. Determine the node of a particle in the states corresponding to n = 1 and n = 2.

(b) Attempt **any one** of the following:-

(i) The Hermite polynomial are derived from the generating function. **04**

$$H_n(y) = (-1)e^n e^{y^2}\frac{d^n}{dy^n}\left(e^{-y^2}\right)$$

where 'n' is the vibrational quantum number and also degree of polynomial. Calculate the polynomials for n = 1 and n = 2

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(ii) Which of the following functions are eigen functions for the operator $\frac{d^2}{dx^2}$? **04**

a) 3 Sin 4 x b) $3e^{-5x}$

2. (a) Attempt **any two** of the following:-

(i) Write the Schrodinger equation in terms of spherical coordinates. Sketch qualitatively the radial distribution functions for 2s and 3s orbitals **04**

(ii) Write only the expressions for total wave function for 1s, 2s, 2p and 3d orbitals of hydrogen. **04**

(iii) Explain the need for approximate solution to two electron system. Show how the problem of two electron can be reduced to problem of one electron system. **04**

(iv) What are quantum numbers? Explain the significance of magnetic quantum number. **04**

(b) Attempt **any one** of the following:-

(i) Calculate the most probable distance of an electron from the nucleus in ground state of hydrogen atom. The normalized ground state function is **04**

$$\psi_{1s} = \frac{1}{\sqrt{\pi}\ a_0^{3/2}} e^{-r/a_0}$$

(ii) The inter nuclear distance between carbon and oxygen atom in CO molecule is 1.13×10^{-10} m. What is the rotational energy for J = 3? **04**

3. (a) Attempt **any two** of the following:-

(i) Explain in brief the Rice-Ramsperger Kassel Marcus (RRKM) theory. **04**

(ii) Discuss the gas phase combustion reaction between H_2 and O_2. Explain the term explosion limits and factors affecting it. **04**

(iii) Explain the kinetics of free radical chain polymerization. **04**

(iv) Explain the mechanism of decomposition of ethane. **04**

(b) Attempt **any one** of the following:-

(i) The following data were obtained for a given reaction at 300K. **04**

Reaction	Energy of activation, kJ mol^{-1}
1. Uncatalyzed	76
2. Catalyzed	57

Calculate by what factor the rate of catalyzed reaction is increased?

(ii) In a bimolecular reaction, the energy of activation is 180 kJ mol^{-1} at 400K. Calculate the specific reaction rate at 400K, if the number of molecules colliding per cc per sec are 6×10^{31}. (R = 8.314 JK^{-1} mol^{-1}) **04**

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4. (a) Attempt **any two** of the following:-

(i) Derive an expression for the contracting area rate law of kinetics of reactions in solid state. **04**

(ii) Discuss the kinetics of enzyme inhibition by non-competitive inhibition method. **04**

(iii) Discuss Eadie-Hoftsee's plot for analysis of the rate data of enzyme catalyzed reaction. **04**

(iv) Discuss the effect of substituents on reaction rate by Hammett's relationship. **04**

(b) Attempt **any one** of the following:-

(i) Calculate the concentration of a non-competitive inhibitor (k_I= 2.5x10^{-4} mol dm^{-3}) needed to yield 60% inhibition of an enzyme catalyzed reaction. **04**

(ii) Predict the effect of ionic strength on the rate constant for each of the following reactions:- **04**

1. $[PtCl_4]^{2-} + OH^- \rightarrow$ Products
2. $Fe^2 + [Co(C_2O_4)_3]^{3-} \rightarrow$ Products
3. $S_2O_8^{2-} + I^- \rightarrow$ Products
4. $CH_2ICOOH + CNS^- \rightarrow$ Products

5. Attempt **any four** of the following:- **12**

(a) Write the applications of Schrodinger's wave equation (any three)

(b) If $\psi = e^{ix}$ and ϕ = sinx, then show that the operator $\frac{d^2}{dx^2}$ is Hermitian.

(c) Explain the statement 'There is an equal chance of finding 1s electron in any direction with respect to nucleus'.

(d) Give the physical significance of spherical harmonics.

(e) State the limitations of the collision theory.

(f) Explain consecutive reactions with examples.

(g) Discuss the various factors affecting reactions in solids.

(h) Write a note on enzyme activation by metal ions.
