St. Joseph's College of Arts & Science (Autonomous)
Cuddalore – 607001

QUESTION BANK

CLASS: I - M.Sc., CHEMISTRY, SEMESTER-I

SUBJECT: QUANTUM MECHANICS AND MOLECULAR STRUCTURE

SUBJECT CODE: PCH703T

UNIT : I

1-marks

1. --------is the mathematical representation of Uncertainty principle.
2. Compton effect can be represented as ----------.
3. Hermitian operator can be represented as ---------.
4. Write Schrodinger wave equation.
5. The expectation value of an operator is ----------.
6. The value of permittivity of the medium is -------
7. Among the following which is a real quantity.a)Ψ^2,b) $\Psi^*\Psi$, c) both a and b, d) none of these.
8. Uncertainty in position of an electron (mass=9.1×10^{-28} g) moving with a velocity of 3×10^4 cm/s accurate up to 0.001% will be _____
9. Photoelectric emission is observed from a surface for frequencies ν_1 and ν_2 of incident radiations ($\nu_1 > \nu_2$). If the maximum kinetic energy of photoelectrons in the two cases are in the ratio of 1:2, then threshold frequency $\nu 0$ is given by _____
10. The amount of energy required to remove the electron from a Li^{2+} ion in its ground state is how many times greater than the amount of energy needed to remove the electron from an H atom in its ground state?
11. The energy of an electron moving I n^{th} Bohr's orbit of an element is given by $E_n = -13.6/n^2Z^2$ eV/atom. The graph of E vs Z^2 (keeping 'n' constant)will be_____
12. If the radius of 2^{nd} Bohr orbit of hydrogen atom is r_2. The radius of 3^{rd} Bohr orbit will be _____
13. Energy required to stop the ejection of electron from Cu plate is 0.24 eV. Calculate the work function when radiation of λ = 253.7 nm strikes the plate.
14. Energy for 7.25×10^{15} photons of 5.37×10^{14} s^{-1} frequency in Einstein unit is _____
15. Number of waves made by a Bohr electron in one complete revolution in 3^{rd} orbit is

2-MARKS :

1. State Compton effect.
2. State Uncertainity principle.
3. Define an Operator with example.
4. Define Eigen function & Eigen value with example.
5. How does an Operator shows Commutative property ?
6. Define Commutator operator with example.
7. Write Hamiltonian operator for Hydrogen molecule in atomic units.
8. A Tennis ball weighing 100 g is to be located within 0.1 Å. What is the uncertainity inb its velocity? Comment your result.
9. Calculate the Compton shift when ( ) is a) 90® & b) 180®.
10. What the degeneracy of the particle in 3D box when nx, ny, nz values were a) (1,1,3) b) (1,2,3) respectively.
11. Calculate for E111 & E112 for particle in 3D box.
12. Calculate the de-Broglie wavelength of elctron moving with a velocity of 1.20×105 ms-1.
13. The emission spectrum of H atom is analysed between 100 nm and 400 nm. What spectral lines are seen in this region?
14. Calculate the Wavelength of an electron (m=9.1×10-31Kg) having energy equal to 1000Ev in SI units.
15. If the position of the electron (m=9.1×10-31Kg) in H atom could be determined with an accuracy of 0.001nm, what would the uncertainity in its velocity? Comment on results.
16. Calculate the width of the spectral lines resulting when an atom in an excited state of life tie 10-10 s returns to the ground state.
17. The equation for a standing wave in a string has the form φ (x,t) = φ(x).cos(ωt), a) calculate the time-averaged potential energy and kinetic energy for this motion. b) Show that E$\propto$ φ2(x).
18. Indicate which of the following functions are acceptable has wave functions : a) $\varphi = x$ b)$\varphi = x2$ c) φ=sin x d) φ=e-x e) φ = ex2 f) φ= tan x

19. Find the eigen function and eigen values of linear momentum operators px, Show that in the absence of any restriction there is a continous series of eigen values of px.

20. Calculate the wavelength of an electron in an H atom in the ground state.

21. Prove $A\varphi = \lambda\varphi$ is linear.

22. Verify the operator ∇2+∇ is linear.

8-MARKS :

1. Discuss the postulates of Quantum mechanics.
2. Explain Bohr's quantum theory.
3. Derive the energy relation and Schrodinger equation for a Particle in a ID box.
4. Derive the energy relation and Schrodinger equation for a Particle in a 3D box.
5. Explain the properties of Operator.
6. Derive the energy relation and Schrodinger equation for a particle in a 2D box.
7. For a particle in a cubic box of edge L, a) How many states have energy in the range 0 to 16 h2/8mL2 b) How many energy levels lie in this range. c) Draw the energy level diagram including degenerates states.
8. Calculate the most probable distance rm of an electron in the 2p state of H atom.
9. Normalize the following functions: a) φ=e-r b) φ=re-r2 cosθ
10. Which of the functions sin3x, 6cos4x, $5x^3$, 1/x, $3e^{-5x}$, ln2x, are eigen functions of d^2/dx^2 ? For each eigen function state eigen value.

UNIT : II

1. Time period τ=-------.a)2πω, b) 2π/ω, c) 2ω/π, d) πω
2. Among the following which is true for a particle in a ring.a)x=rcosϕ, b) y=rsinϕ, c) x= cosϕ, d) both a and b.

2-MARKS :

1. State Hook's law.
2. What are Harmonic oscillator?
3. Write the Schrodinger equation for a rigid diatomic molecule if it rotates in a fixed axis.

4. Write the Schrodinger equation for hydrogen atom.
5. Draw the potential energy diagram for Simple harmonic oscillator.
6. Write the Eigen value for Rigid rotor.
7. Write the Eigen value for Rigid rotor in terms of I & J.
8. What is the maximum probability density for a ID simple harmonic oscillator in the ground vibrational state?
9. Write the Schrodinger equation for particle in a ring.
10. Write the Schrodinger equation for a rigid diatomiv molecule if it rotates in a free axis.
11. What is the kinetic energy relation for a diatomic molecule when its rotates ?

8-MARKS :

1. Write a note on quantum mechanical treatment of a harmonic oscillator.
2. Write the Schrodinger's equation for Simple harmonic oscillator. Derive its Eigen function & Eigen value.
3. Write the Schrodinger's equation for particle in a ring. Derive its Eigen function & Eigen value.
4. Write the Schrodinger's equation for rigid rotator. Derive its Eigen function & Eigen value.
5. The rotation of an HI molecule may be considered of the H atom at a radius of 160 pm with I virtually stationary at the center, Determine the energy levels considering the rotation to be restricted. a) in x-y plane and b) in 3D. Indicate the degeneracies of the energy levels . What will be the wavelength of rotation emitted for transition from the first excited to the ground state in either case.

UNIT: III

2-MARKS

1. Write the principle of Variation method.
2. What is the energy relation for H_2 molecule based on LCAO-MO?
3. State the Born Oppenheimer approximation.
4. For which type of system the perturbation method is applied ?
5. Calculate the term symbol for N2 molecule, Cr^{2+}, Ne, He, Mn^{2+}.

8-MARKS

1. Discuss perturbation theory.
2. Explain Variation method.
3. Explain how Huckel theory is used to explain hybridization in Ethylene.
4. Explain how Huckel theory is used to explain hybridization in Butadiene.
5. Explain how Huckel theory is used to explain hybridization in Benzene.
6. Explain the LCAO-MO approximation for Hydrogen molecule.
7. Use the Trial function $\Psi=\exp^{(-ar2)}$ (without the normalization factor) for the ground state of the hydrogen atom. a) Apply variation method to find the value of α that would give the minimum energy. b) Determine that energy. c) Calculate the average value of r and the most probable value of r using this wave function. d) What is the normalization factor?
8. A Hydrogen atom is exposed to an electric field of strength F applied in the z-direction. Calculate the first order and the second order effects for the ground state of the atom (Strak effect).
9. Use a trial function, $\Psi=Nre^{-ar}$ to calculate the ground state energy of the H atom. Compare the result with the true value. Also determine the Value of N.
10. An electron moving in a simple Harmonic potential Y= ½ Kx2 is subjected to a perturbation $\hat{H}$=Ex, where E is the strength of the electric field which is applied in the x-direction. Determine the effect of first and second order perturbation on the energy.

UNIT-IV

2-MARKS

1. Write the postulates of FMO theory.
2. Write the HMO equation for Butadiene
3. What is the importance of Walsh diagram?
4. Explain Zeeman effect.
5. Using Walsh diagram predict the geometry of BeH_2 , CH_2 & H_2O.
6. Write the normalized wave function for Ethylene & Butadiene
7. Calculate the HOMO-LUMO energy gap for ethylene & Butadiene as per Huckel's method

5-MARKS

1. Explain the assumptions of Huckel method.
2. Explain the FMO theory for Benzene.
3. Explain the FMO theory for Naphthalein.
4. Explain the FMO theory for Butadiene.
5. Explain the FMO theory for Cyclobutadiene.

UNIT: V

2-MARKS

1. What are Slater orbitals ?
2. Write Hartree equation for radial function.
3. Write the Fock matrix and overlap matrix in Roothaan's equation.
4. Write slater rule.

5-MARKS

1. Derive Roothan's equation.
2. Explain Hartree-Fock consistent field method for polyatomic molecule.
3. Discuss Slater rule.
4. Calculate the effective nuclear charge for the 2s electron in Li atom, given that the first ionization potential is 5.4 eV.
5. Sketch the radial function for 1s atomic orbitals of He+ ion and He atom and compare.
6. Write the ground state configuration and calculate the screening constant and the effective nuclear charge for the following Slater's rule.
    a) 2s & 2p electrons of C and N
    b) 3s & 3p electrons of S
    c) 1s electrons of F