

K21P 0518

Reg. No. :

Name :

**First Semester M.Sc. Degree (CBSS – Reg./Supple. (Including Mercy
Chance)/Imp.) Examination, October 2020
(2014 Admission Onwards)
CHEMISTRY
CHE 1C.01 : Theoretical Chemistry – I**

Time : 3 Hours

Max. Marks : 60

SECTION – A

Answer **all** questions in **one word** or **sentence**. Each question carries **1** mark.
(8×1=8)

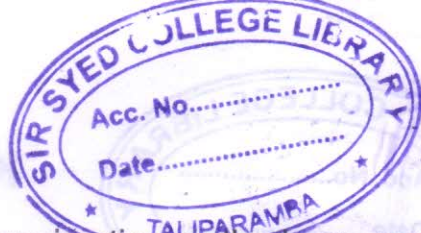
1. What is Compton effect ?
2. What is linear operator ? Give one example.
3. Write down the Hamiltonian operator in spherical polar coordinates.
4. What is a node and how it varies with quantum number in Particle in a 1-D box problem ?
5. What is the nature of the wave function proposed by Hartree ?
6. Write down the perturbation term in Helium atom.
7. What is Born Oppenheimer approximation ?
8. Write down the Schrodinger equation for an n-electron, N-nuclei molecule.

SECTION – B

Answer **eight** questions. Answer may be **two** or **three** sentences. Each question carries **2** marks.
(8×2=16)

9. Expand the operator $(x \cdot d/dx)^2$.
10. Prove that Hermitian operators have real eigen values.
11. Give a trigonometric function that is an eigen function of both d/dx and d^2/dx^2 .
12. Explain transition moment integral and indicate its importance.
13. What are polar diagrams ?
14. What is the form of Laguerre equation ?

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15. Why approximation methods are required to solve the Schrodinger equation of many electron systems ?
16. Write down the ground state term symbol for a) C-atom b) N-atom.
17. Draw the radial distribution functions of 1s, 2s, 3p and 3d.
18. What is meant by 'ab initio method' ? Give an example.
19. What is STO ? State its two limitations.
20. How do you calculate free valence index ? Mention its importance.

SECTION - C

Answer **four** questions in short paragraph for **each**. **Each** question carries **3** marks.

(4×3=12)

21. A system is defined by the wave function $\psi(x) = \cos(2\pi x/L)$ with x varies between $-L/4$ and $L/4$. Normalize the wave function and find out the probability of the particle that will be found between $x = 0$ and $x = L/8$.
22. Prepare the Hermite polynomial, $H_5(x)$ and write down the simple harmonic wave function $\psi_5(x)$.
23. Starting from time dependent Schrodinger equation, arrive at the time independent form by separating the variables.
24. Explain tunneling effect.
25. Explain 'Self consistent field' method.
26. What is a basis set ? Explain the various classifications of basis sets.
27. What are the approximations incorporated in Huckel molecular orbital treatment of conjugated systems.
28. Draw the molecular orbital diagram for O_2 molecule. Extend this to O_2^+ and O_2^- and calculate the bond orders.

SECTION - D

Answer either **a** or **b** of **each** question. **Each** question carries **6** marks.

(4×6=24)

29. a) Explain the main postulates of quantum mechanics.

OR

- b) Name three experimental phenomena where classical mechanics failed. Also explain, how quantum mechanics explained these satisfactorily.



30. a) Write down the exact wave function form of non planar rigid rotor. With the help of this, justify the various quantum number values of 'l' and 'm'.

OR

- b) Starting from the Schrodinger equation of hydrogen atom in spherical polar coordinates, separate the variables and arrive at single variable equations. Also, derive the energy expression.

31. a) Solve for variational parameter α and energy if the trial wave function proposed for hydrogen atom is $e^{-\alpha r}$.

OR

- b) Solve the first order perturbation equation for a non-degenerate system to arrive at first order correction to energy.

32. a) Solve the Schrodinger equation of H_2 molecule under molecular orbital theory.

OR

- b) Arrive at the molecular term symbols of O_2 and arrange them in the order of energy.

