QP Code: D133772	Total Pages:1	Name: 664380
		Register No.

THIRD SEMESTER UG DEGREE EXAMINATION, NOVEMBER 2025

(CUFYUGP)

CHE3CJ 201 - THEORETICAL CHEMISTRY I – BASIC QUANTUM CHEMISTRY

2024 Admission onwards

Maximum Time :2 Hours | **Maximum Marks :70**

Section A

All Questions can be answered. Each Question carries 3 marks (Ceiling : 24 Marks)

1	State Planks quantum theory.
2	Explain why classical physics failed to explain black body radiation?
3	Describe the experimental observations of the photoelectric effect.
4	State the two main postulates of Bohr's atomic model and explain how they differ from Rutherford's model.
5	How does Bohr's model explain the spectral lines of hydrogen?
6	State the Heisenberg's uncertainty principle.
7	State the postulate of the time-dependent Schrödinger wave equation.
8	Explain why eigenfunctions of the Hamiltonian operator must be normalised.
9	What is hybridisation?
10	Why CH_4 is tetrahedral?

Section B

All Questions can be answered. Each Question carries 6 marks (Ceiling : 36 Marks)

11	Derive the photoelectric equation $h\nu=h\nu_0+KE$ using Einstein's quantum theory of light.
12	Explain how the energy levels of a particle in a 1D box with finite potential walls differ from those with infinite walls.
13	What is quantum tunnelling? Explain with an example from nuclear or electronic processes.
14	Define an atomic orbital as a wavefunction. Distinguish between its radial and angular parts.
15	State and explain Paulis exclusion principle.
16	Write the Hamiltonian operator for the hydrogen molecule (H_2). Identify the terms representing electron kinetic energy, nuclear kinetic energy, and potential energy contributions.
17	State the Born–Oppenheimer approximation. Why is it valid to separate nuclear and electronic motions in molecules?
18	Explain the bonding and hybridisation of PCl_5.

Section C

Answer any ONE .Each Question carries 10 marks (1x10=10 Marks)

19	Derive the wave functions and energy of a particle in a one-dimensional box with infinite potential energy walls .
20	Draw Molecular orbital energy diagram of CO and NO . Compare bond order and magnetism.