

QP CODE: D3BCH2401

(Pages: 2)

Reg. No :

Name :

THIRD SEMESTER FYUGP EXAMINATION, NOVEMBER 2025

Discipline Specific Core (DSC) Courses - Major

CHE3CJ201 : THEORETICAL CHEMISTRY- I: BASIC QUANTUM CHEMISTRY

(Credits: 4)

Time: 2 Hours

Maximum Marks: 70

Section A**Answer the following questions. Each carries 3 marks (Ceiling: 24 marks)**

1.	What is Plank's quantum hypothesis?	BL1	CO1
2.	Explain the Born interpretation of wave function.	BL2	CO2
3.	Explain the terms (i) Laplacian operator and (ii) Hamiltonian operator.	BL2	CO2
4.	Explain with an example what is meant by degeneracy of energy levels in a cubic box.	BL3	CO2
5.	Explain why the ground-state energy of a particle in a 1D box is not zero.	BL4	CO2
6.	Write the Hamiltonian operator for a hydrogen-like atom in spherical polar coordinates and briefly explain each term.	BL1	CO2
7.	What is meant by electron spin? How was it discovered?	BL2	CO2
8.	What is Born-Oppenheimer approximation?	BL2	CO3
9.	What is the significance of the minimum point in the potential energy curve of H ₂ formation?	BL2	CO3
10.	Write the mathematical expressions of sp ² hybrid orbital.	BL2	CO4

Section B**Answer the following questions. Each carries 6 marks (Ceiling: 36 Marks)**

11.	Give the expression for the radius of Bohr orbit as well as the velocity and energy of an electron in a hydrogen atom, explaining the terms involved.	BL3	CO1
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12.	Sketch the energy level diagram for particle in a 1D box. How is the particle-in-a-box model applied to explain the absorption band in 1,3-butadiene?	BL3	CO2
13.	Give a concise explanation of the quantum numbers n, l, and m associated with the hydrogen atom.	BL2	CO2
14.	State the eigenvalue postulate in quantum mechanics. Show that Hermitian operators have real eigen values.	BL2	CO2
15.	Show mathematically that if two electrons have the same set of quantum numbers, the total wavefunction vanishes.	BL3	CO2
16.	Discuss the characteristics of the different types of sigma molecular orbitals.	BL2	CO3
17.	Draw the MO energy diagram for CO molecule. Calculate the bond order and explain its stability and magnetic behaviour.	BL3	CO3
18.	Define hybridization .Explain the wave mechanical basis of the formation of hybrid orbitals taking the example of sp hybridization.	BL2	CO4

Section C

Answer any one question. Each carries 10 marks (1 x 10 = 10 Marks)

19.	Explain how de Broglie's hypothesis and the Davisson–Germer experiment provided further evidence for the wave nature of matter.	BL2	CO1
20.	Discuss the origin of tunnelling in a particle confined to a one-dimensional box with finite potential walls. Highlight its physical significance with examples.	BL2	CO2

CO : Course Outcome

BL : Bloom's Taxonomy Levels (1 – Remember, 2 – Understand, 3 – Apply, 4 – Analyse, 5 – Evaluate, 6 – Create)